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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	May 12	EXTEND option available in structure searching
NEWS 4	May 12	Polymer links for the POLYLINK command completed in REGISTRY
NEWS 5	May 27	New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus
NEWS 6	May 27	CAplus super roles and document types searchable in REGISTRY
NEWS 7	Jun 28	Additional enzyme-catalyzed reactions added to CASREACT
NEWS 8	Jun 28	ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG, and WATER from CSA now available on STN(R)
NEWS 9	Jul 12	BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS
NEWS 10	Jul 30	BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting
NEWS 11	AUG 02	IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields
NEWS 12	AUG 02	CAplus and CA patent records enhanced with European and Japan Patent Office Classifications
NEWS 13	AUG 02	STN User Update to be held August 22 in conjunction with the 228th ACS National Meeting
NEWS 14	AUG 02	The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available
NEWS 15	AUG 04	Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004
NEWS 16	AUG 27	BIOCOMMERCE: Changes and enhancements to content coverage
NEWS 17	AUG 27	BIOTECHABS/BIOTECHDS: Two new display fields added for legal status data from INPADOC

NEWS EXPRESS	JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that specific topic.

* * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 08:07:21 ON 01 SEP 2004

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 08:07:37 ON 01 SEP 2004

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 30 AUG 2004 HIGHEST RN 736108-36-4
DICTIONARY FILE UPDATES: 30 AUG 2004 HIGHEST RN 736108-36-4

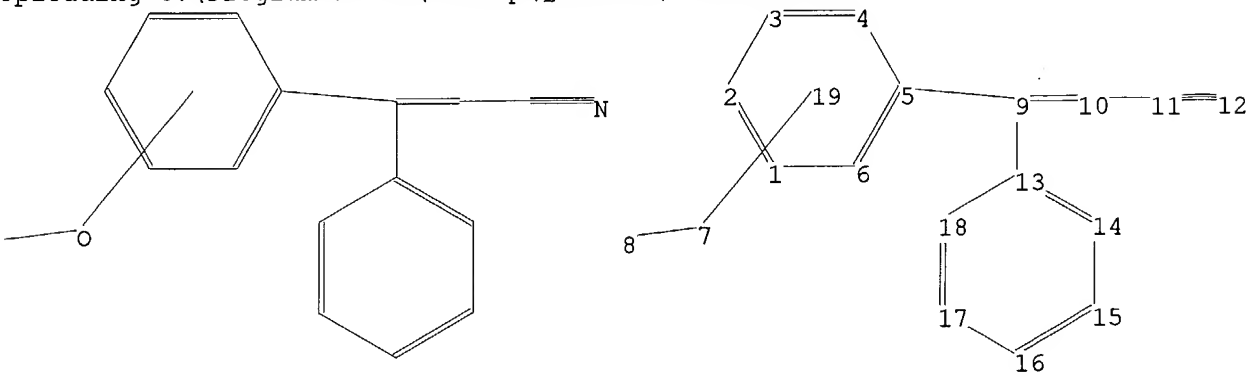
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10622618.str



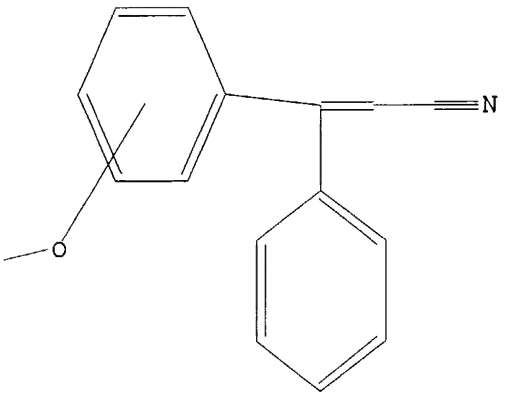
chain nodes :
7 9 10 11 12
ring nodes :
1 2 3 4 5 6 13 14 15 16 17 18
ring/chain nodes :
8
chain bonds :
5-9 7-8 9-10 9-13 10-11 11-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
exact/norm bonds :

7-8 11-12
exact bonds :
5-9 9-10 9-13 10-11
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 08:07:50 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 85 TO ITERATE

100.0% PROCESSED 85 ITERATIONS 11 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 1147 TO 2253
PROJECTED ANSWERS: 22 TO 418

L2 11 SEA SSS SAM L1

=> s l1 full
FULL SEARCH INITIATED 08:07:53 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 1748 TO ITERATE

100.0% PROCESSED 1748 ITERATIONS 224 ANSWERS
SEARCH TIME: 00.00.01

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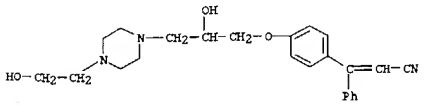
L3          224 SEA SSS FUL L1

=> s l3 and caplus/lc
      38360223 CAPLUS/LC
L4          212 L3 AND CAPLUS/LC

=> s l3 not l4
L5           12 L3 NOT L4

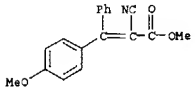
=> d l5 1-12
```

L5 ANSWER 1 OF 12 REGISTRY COPYRIGHT 2004 ACS on STN
RN 708200-33-3 REGISTRY
CN 2-Propenenitrile, 3-[4-[2-hydroxy-3-[4-(2-hydroxyethyl)-1-piperazinyl]propoxy]phenyl]-3-phenyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C24 H29 N3 O3
CI COM
SR CA



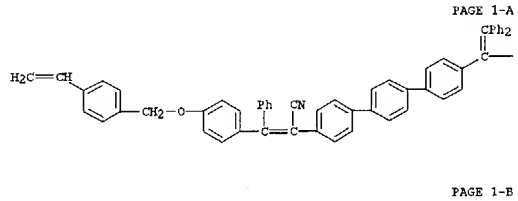
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 2 OF 12 REGISTRY COPYRIGHT 2004 ACS on STN
RN 408537-44-0 REGISTRY
CN 2-Propenoic acid, 2-cyano-3-(4-methoxyphenyl)-3-phenyl-, methyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H15 N O3
SR Reaction Database
LC STN Files: CASREACT



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 3 OF 12 REGISTRY COPYRIGHT 2004 ACS on STN
RN 326592-62-5 REGISTRY
CN [1,1':4',1''-Terphenyl]-4,4''-diacetonitrile, α-(diphenylmethylene)-α'-[[4-[(4-ethenylphenyl)methoxy]phenyl]phenylmethylene]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C57 H40 N2 O
CI COM
SR CA



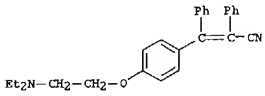
PAGE 1-A

PAGE 1-B

—CN

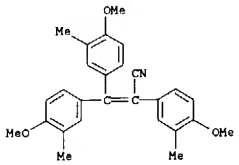
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 4 OF 12 REGISTRY COPYRIGHT 2004 ACS on STN
RN 207562-97-8 REGISTRY
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl]phenylmethylene]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C27 H28 N2 O
CI COM
SR CA



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 5 OF 12 REGISTRY COPYRIGHT 2004 ACS on STN
RN 114695-45-3 REGISTRY
CN Acrylonitrile, 2,3,3-tris(4-methoxy-m-tolyl)- (6CI) (CA INDEX NAME)
FS 3D CONCORD
MF C27 H27 N O3
SR CAOLD
LC STN Files: CAOLD

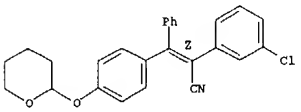


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L5 ANSWER 6 OF 12 REGISTRY COPYRIGHT 2004 ACS on STN
RN 19605-72-2 REGISTRY
CN Acrylonitrile, 2-(p-chlorophenyl)-3-phenyl-3-[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]-, (Z)- (8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H22 Cl N O2

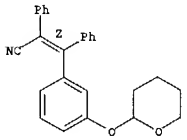
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 7 OF 12 REGISTRY COPYRIGHT 2004 ACS on STN
RN 19460-08-3 REGISTRY
CN Acrylonitrile, 2,3-diphenyl-3-[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]-, (Z)- (8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C26 H23 N O2

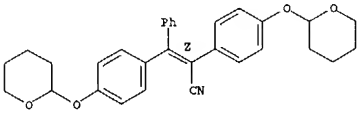
Double bond geometry as shown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

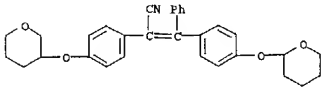
L5 ANSWER 8 OF 12 REGISTRY COPYRIGHT 2004 ACS on STN
RN 19460-04-9 REGISTRY
CN Acrylonitrile, 3-phenyl-2,3-bis[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]-, (Z)- (8CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H31 N O4
LC STN Files: BEILSTEIN*
(*File contains numerically searchable property data)

Double bond geometry as shown.



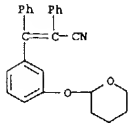
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 9 OF 12 REGISTRY COPYRIGHT 2004 ACS on STN
RN 19094-20-3 REGISTRY
CN Benzeneacetonitrile, α-[phenyl[4-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]methylene]-4-[(tetrahydro-2H-pyran-2-yl)oxy]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C31 H31 N O4



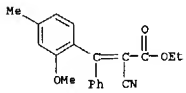
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 10 OF 12 REGISTRY COPYRIGHT 2004 ACS on STN
RN 19001-15-1 REGISTRY
CN Acrylonitrile, 2,3-diphenyl-3-[m-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]- (8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C26 H23 N O2



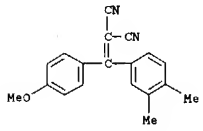
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 11 OF 12 REGISTRY COPYRIGHT 2004 ACS on STN
RN 17212-43-0 REGISTRY
CN Cinnamic acid, α-cyano-2-methoxy-4-methyl-β-phenyl-, ethyl ester (8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H19 N O3



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L5 ANSWER 12 OF 12 REGISTRY COPYRIGHT 2004 ACS on STN
RN 16173-35-6 REGISTRY
CN Malononitrile, [(p-methoxyphenyl)(3,4-xylyl)methylene]- (8CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H16 N2 O



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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COST IN U.S. DOLLARS                                    SINCE FILE      TOTAL
                                                           ENTRY    SESSION
FULL ESTIMATED COST                                       181.93     182.14

FILE 'CAPLUS' ENTERED AT 08:09:35 ON 01 SEP 2004
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 1 Sep 2004  VOL 141 ISS 10
FILE LAST UPDATED: 31 Aug 2004  (20040831/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.


=> s l4
L6          146 L4

=> d ibib abs hitstr 1-146
```
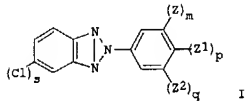

L6 ANSWER 1 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:509928 CAPLUS
DOCUMENT NUMBER: 139:86116
TITLE: Resin composition with cyanoacrylate and benzotriazole UV light absorbers
INVENTOR(S): Abe, Takashi; Kanoh, Kenichiro
PATENT ASSIGNEE(S): Tokuyama Corporation, Japan
SOURCE: Eur. Pat. Appl., 25 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1323743	A2	20030702	EP 2002-258937	20021224
EP 1323743	A3	20031008		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2003253140	A2	20030910	JP 2002-351653	20021203
US 2003176542	A1	20030918	US 2002-325961	20021223
CN 1428365	A	20030709	CN 2002-128169	20021227
PRIORITY APPLN. INFO.:			JP 2001-396149 A	20011227

OTHER SOURCE(S): MARPAT 139:86116
GI



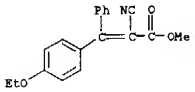
I

AB A resin composition contains a cyanoacrylate UV absorber (a) RxH2-xC:C(CN)CO2R1, where R = aryl group, R1 = organic group having 1-12 C atoms, and x = 1 or 2, and benzotriazole UV absorber I, where Z, Z1 and Z2 = H or organic groups having 1-20 C atoms, and m, p, q and s = 0 or 1. The resin composition possesses light resistance of a satisfactory level even when it is used in optical lenses, developing little yellow color after extended periods of time. Example synergistic stabilizers were Ph2C:C(CN)CO2Et and I (Z2 = Me; Z,Z1 = H; s = 0; m, p, q = 1).

IT **551959-21-8**
RL: MOA (Modifier or additive use); USES (Uses)
(UV stabilizer; lens material with cyanoacrylate and benzotriazole UV light absorbers)

RN 551959-21-8 CAPLUS
CN 2-Propenoic acid, 2-cyano-3-(4-ethoxyphenyl)-3-phenyl-, methyl ester (9CI) (CA INDEX NAME)

L6 ANSWER 1 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

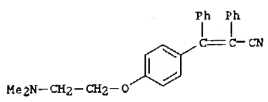


L6 ANSWER 2 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:280572 CAPLUS
DOCUMENT NUMBER: 139:85065
TITLE: Synthesis of α-hydroxytamoxifen and its 4-hydroxy analog
AUTHOR(S): Lashley, M. R.; Dicus, C. W.; Brown, K.; Nantz, M. H.
CORPORATE SOURCE: Department of Chemistry, University of California, Davis, CA, 95616, USA
SOURCE: Organic Preparations and Procedures International (2003), 35(2), 231-238
CODEN: OPPIAK; ISSN: 0030-4948
PUBLISHER: Organic Preparations and Procedures, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:85065

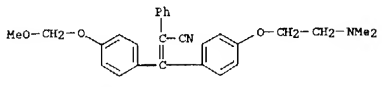
AB New syntheses of α-hydroxytamoxifen and α-hydroxy-4-hydroxytamoxifen via phenylacetonitrile condensation are described.

IT **556834-75-4P 556834-79-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of α-hydroxytamoxifen and its 4-hydroxy analog via condensation)

RN 556834-75-4 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(dimethylamino)ethoxy]phenyl]phenylmethylene]- (9CI) (CA INDEX NAME)



RN 556834-79-8 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(dimethylamino)ethoxy]phenyl][4-(methoxymethoxy)phenyl]methylene]- (9CI) (CA INDEX NAME)



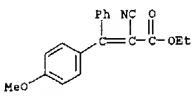
REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 3 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:102664 CAPLUS
DOCUMENT NUMBER: 139:85183
TITLE: Synthesis of 3,3-diarylpyrrolidines from diaryl ketones
AUTHOR(S): Katritzky, Alan R.; Nair, Satheesh K.; Witek, Rachel M.; Hutchins, Steven M.
CORPORATE SOURCE: Center for Heterocyclic Compounds, Dept. of Chem., Univ. of Florida, Gainesville, FL, 32611-7200, USA
SOURCE: ARKIVOC (Gainesville, FL, United States) (2003), (5), No pp. given
CODEN: AGFUAR
URL: http://www.arkat-usa.org/zark/journal/2003/Bernath/GB-594J/594J.pdf
PUBLISHER: Arkat USA Inc.
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:85183

AB 3,3-Diarylsuccinic acids were prepared from diaryl ketones by the Knoevenagel condensation with Et cyanoacetate followed by KCN addition and hydrolysis. These were cyclized using primary amines to the resp. diarylpyrrolidones, which were finally reduced to 3,3-diarylpyrrolidines using BH3THF.

IT **14442-38-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; synthesis of diarylpyrrolidines from diaryl ketones in multi-step procedure)

RN 14442-38-7 CAPLUS
CN 2-Propenoic acid, 2-cyano-3-(4-methoxyphenyl)-3-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

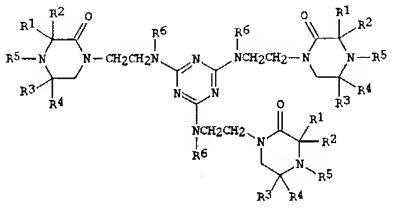


REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 4 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:5031 CAPLUS
DOCUMENT NUMBER: 138:75925
TITLE: Stabilization of candle wax with UV stabilizers, antioxidants, and piperazinones
INVENTOR(S): Wood, Mervin G.; Smith, Andrea R.; Judd, Deborah
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 12 pp., Cont.-in-part of U.S. Ser. No. 824,194.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003000130	A1	20030102	US 2002-93111	20020307
US 2002194777	A1	20021226	US 2001-824194	20010402
US 6544305	B2	20030408		
PRIORITY APPLN. INFO.:			US 2001-824194	A2 20010402

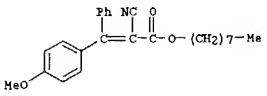
OTHER SOURCE(S): MARPAT 138:75925
GI



I

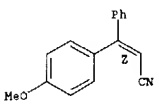
AB White, dyed, dipped, and unscented (or scented) candle wax is stabilized by a mixture of a UV absorber (and/or antioxidant) and a piperazinone compound of general structure I, in which: (1) R1-4 = C1-12-alkyl, hydroxyalkyl, or adjacent R (e.g., R1R2 or R3R4) is a spiro-6-8-membered cycloalkyl ring, (2) R5 = H, OH, CH2CH2CN, C7-15-phenylalkyl, C7-15-alkoxyalkyl, C1-4-alkoxy, C5-12-cycloalkoxy, C3-8-alkenyl or -alkynyl, C2-18-alkylcarbonyloxy, C1-8-alkanoyl, C3-5-alkenoyl, or 4-hydroxy-3,5-di-tert-butylbenzoyloxy, and (3) R6 = C1-8-alkyl or -alkanoyl, C5-12-cycloalkyl, C7-15-phenylalkyl. Suitable UV absorbers include a benzotriazole, a benzophenone, an α-cyanoacrylate, an oxanilide, an s-triazine, a cinnamate ester, a malonate or methylenemalonate. The candle wax compns. are stabilized against discoloration and fading.
IT **481019-30-1**

L6 ANSWER 4 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RL: MOA (Modifier or additive use); USES (Uses)
(antioxidant-UV stabilizer; stabilization of candle wax with UV stabilizers, antioxidants, and piperazinones)
RN 481019-30-1 CAPLUS
CN 2-Propenoic acid, 2-cyano-3-(4-methoxyphenyl)-3-phenyl-, octyl ester (9CI) (CA INDEX NAME)



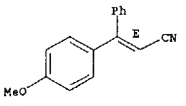
L6 ANSWER 5 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:790736 CAPLUS
DOCUMENT NUMBER: 138:187193
TITLE: Stereospecific synthesis of 3,3-disubstituted acrylonitriles by Heck reaction
AUTHOR(S): Masllorens, Judit; Moreno-Manas, Marcial; Pla-Quintana, Anna; Pleixats, Roser; Roglans, Anna
CORPORATE SOURCE: Department of Chemistry, Universitat de Girona, Girona, 17071, Spain
SOURCE: Synthesis (2002), (13), 1903-1911
CODEN: SYNTBF; ISSN: 0039-7881
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:187193
AB The coupling reaction of 3-aryl (or heteroaryl) acrylonitriles with several aryl and heteroaryl iodides (Heck reaction) under Jeffery's conditions has been studied as a concept to synthesize, in a stereospecific manner, trisubstituted olefins. E.g., palladium-catalyzed arylation of (E)-cinnamonitrile with 4-iodoaniline gave (E)-4-H2NC6H4CPh:CHCN.
IT **170879-10-4P 170879-13-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereospecific preparation of acrylonitriles by Heck reaction of aryl acrylonitriles with aryl iodides)
RN 170879-10-4 CAPLUS
CN 2-Propenenitrile, 3-(4-methoxyphenyl)-3-phenyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



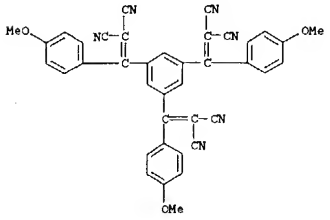
RN 170879-13-7 CAPLUS
CN 2-Propenenitrile, 3-(4-methoxyphenyl)-3-phenyl-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



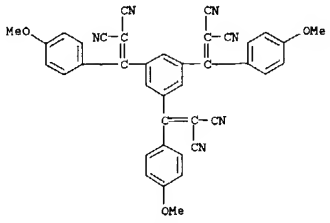
REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 6 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:647708 CAPLUS
DOCUMENT NUMBER: 138:122307
TITLE: Redox and magnetic switching in 1,3,5-acceptor-substituted benzenes: reversible formation of radical anions, dianions and trianions in doublet, triplet, and quartet spin states
AUTHOR(S): Beer, Ernst; Daub, Joerg; Palivan, Cornelia; Gescheidt, Georg
CORPORATE SOURCE: Institute of Organic Chemistry, Universitaet Regensburg, Regensburg, D-93053, Germany
SOURCE: Journal of the Chemical Society, Perkin Transactions 2 (2002), (9), 1605-1610
CODEN: JCSPGI; ISSN: 1472-779X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 1,3,5-Tris(2,2-dicyano-1-phenylvinyl)benzene 1 can accept one, two, and three electrons stepwise, as shown by (spectro)electrochem. methods. When the corresponding redox stages are attained by K-metal reduction in THF and 2-methyltetrahydrofuran, paramagnetic resonance and optical techniques can identify equilibrium between adjacent redox states and different (para)magnetic stages. It can be shown that the dianion can adopt a triplet state whereas the trianion is present in a doublet and quartet spin multiplicity. Similar findings are established for the 4-methoxyphenyl derivative 2. The formation of the different paramagnetic stages is closely connected to the association of the anions with alkali-metal countercations.
IT **489468-31-7 489473-58-7 489473-76-1**
RL: FMU (Formation, unclassified); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); RACT (Reactant or reagent)
(reduction and redox potential; redox and magnetic switching in 1,3,5-acceptor-substituted benzenes with reversible formation of radical anions, dianions and trianions in doublet, triplet, and quartet spin states)
RN 489468-31-7 CAPLUS
CN Propanedinitrile, 2,2',2''-[1,3,5-benzenetriyltris[(4-methoxyphenyl)methylidyne]]tris-, radical ion(1-) (9CI) (CA INDEX NAME)

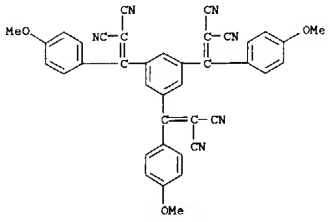


RN 489473-58-7 CAPLUS
CN Propanedinitrile, 2,2',2''-[1,3,5-benzenetriyltris[(4-methoxyphenyl)methylidyne]]tris-, radical ion(2-) (9CI) (CA INDEX NAME)

L6 ANSWER 6 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

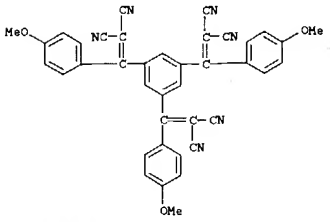


RN 489473-78-1 CAPLUS
CN Propanedinitrile, 2,2',2''-[1,3,5-benzenetriyltris[(4-methoxyphenyl)methylidyne]]tris-, radical ion(3-) (9CI) (CA INDEX NAME)

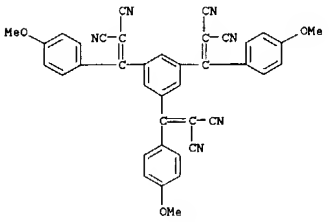


IT **489468-30-6**
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(reduction and redox potential; redox and magnetic switching in 1,3,5-acceptor-substituted benzenes with reversible formation of radical anions, dianions and trianions in doublet, triplet, and quartet spin states)
RN 489468-30-6 CAPLUS
CN Propanedinitrile, 2,2',2''-[1,3,5-benzenetriyltris[(4-methoxyphenyl)methylidyne]]tris- (9CI) (CA INDEX NAME)

L6 ANSWER 6 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT **489468-33-9**
RL: FMU (Formation, unclassified); PRP (Properties); FORM (Formation, nonpreparative)
(redox and magnetic switching in 1,3,5-acceptor-substituted benzenes with reversible formation of radical anions, dianions and trianions in doublet, triplet, and quartet spin states)
RN 489468-33-9 CAPLUS
CN Propanedinitrile, 2,2',2''-[1,3,5-benzenetriyltris[(4-methoxyphenyl)methylidyne]]tris-, radical ion(1-), potassium (9CI) (CA INDEX NAME)



● K+

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 7 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:355087 CAPLUS
DOCUMENT NUMBER: 134:348291
TITLE: Preparation and method for the treatment and prevention of dementia disorders based on antiestrogens
INVENTOR(S): Denecke, Rainer
PATENT ASSIGNEE(S): Altramed Holdings Ltd., Belg.
SOURCE: U.S., 9 pp., Cont.-in-part of U.S. Ser. No. 532,681, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6232350	B1	20010515	US 1997-852274	19970507
DE 4311870	A1	19941013	DE 1993-4311870	19930410
DE 4311870	C2	19980730		
WO 9423708	A1	19941027	WO 1994-DE366	19940330
W: AU, BB, BG, BR, BY, CA, CN, CZ, FI, HU, JP, KP, KR, KZ, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SI, SK, TT, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 2001018434	A1	20010830	US 2001-784615	20010215

PRIORITY APPLN. INFO.:
DE 1993-4311870 A 19930410
WO 1994-DE366 B2 19940330
US 1995-532681 B2 19951208
US 1997-852274 A1 19970507

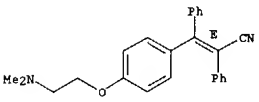
OTHER SOURCE(S): MARPAT 134:348291

AB A composition for the treatment and/or prevention of dementia disorders in humans, especially disorders due to regressive cellular changes, comprises at least one steroidal antagonist, in particular triphenylethylene antiestrogens and derivs. The composition is administered in an amount of 5-100 mg/day for about 3-24 mo. The antiestrogen is selected from the group consisting of tamoxifen or a tamoxifen derivative, such as 3- or 4-hydroxytamoxifen, N-desmethyltamoxifen, monophenoltamoxifen, cyanotamoxifen, CB 7432, toremifene, 4-hydroxytoremifene, N-desmethyltoremifene, monophenoltoremifene, and deaminotoremifene. For example, a male human having a body mass of 72-78 kg was treated with 3-hydroxytamoxifen *(droloxifene) 40 mg/day administered once per day for a period of 6 mo.

IT **339176-84-0**
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compns. containing steroidal antagonists for treatment and prevention of dementia disorders)
RN 339176-84-0 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(dimethylamino)ethoxy]phenyl]phenylmethylene]-, (αE)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L6 ANSWER 7 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 8 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:129765 CAPLUS
DOCUMENT NUMBER: 134:185757
TITLE: Luminescent material and luminescent component
INVENTOR(S): Tsukada, Yoshihisa; Adegawa, Yutaka
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 23 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

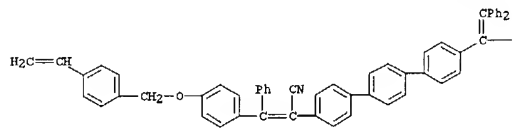
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001049247	A2	20010220	JP 1999-224074	19990806
PRIORITY APPLN. INFO.:			JP 1999-224074	19990806

AB The invention refers to an electroluminescent material and device containing the compound [CH2CR3(L1)q(X1)r(L2)sAr1C(Ar2):CR1Ar3-CR2:C-Ar3Ar4]p [Ar1,3 = arylene, divalent heterocyclic, or a combination thereof; Ar2,4,5 = H, aryl, or heterocyclic; R1,2 = H, cyano, alkyl, alkoxy, alkylthio, aryloxy, arylthio, heterocyclic, oxyheterocyclic, or thioheterocyclic; R3 = H, halo, alkyl, or aryl; p ≥ 1; L1,2 = divalent linking group; X1 = alkylene, arylene, divalent heterocyclic, or -R4(OR5)t-; q,r,s = 0, 1; R4,5 = alkylene; t ≥ 1].
IT **326592-63-6**
RL: DEV (Device component use); USES (Uses)
(luminescent material and luminescent component)
RN 326592-63-6 CAPLUS
CN [1,1':4',1''-Terphenyl]-4,4''-diacetonitrile, α-(diphenylmethylene)-α'-[[4-[(4-ethenylphenyl)methoxy]phenyl]phenylmethylene]-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 326592-62-5
CMF C57 H40 N2 O

PAGE 1-A

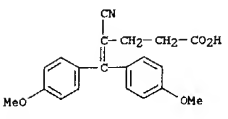


PAGE 1-B

—CN

L6 ANSWER 8 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L6 ANSWER 9 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:43071 CAPLUS
DOCUMENT NUMBER: 135:116844
TITLE: Effect of E5510, a novel antiplatelet agent, on platelet deposition in atherothrombotic lesions: Evaluation by 111In platelet scintigraphy
AUTHOR(S): Moriwaki, H.; Matsumoto, M.; Handa, N.; Hashikawa, K.; Hori, M.; Nishimura, T.
CORPORATE SOURCE: Cerebrovascular Division, National Cardiovascular Center, Osaka, 565-8565, Japan
SOURCE: Nuclear Medicine Communications (2000), 21(11), 1051-1058
CODEN: NMCODC; ISSN: 0143-3636
PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We evaluated the short-term effects of a novel antiplatelet agent, 4-cyano-5,5-bis(methoxyphenyl)-4-pentenoic acid (E5510), using 111In platelet scintigraphy (PSG) and B-mode ultrasonog. (US). Fifteen patients with platelet deposition at either the carotid bifurcation or abdominal aorta on PSG were randomized into two groups: seven were followed without anti-thrombotic medication (Group A) and eight received E5510 (4 mg•day-1) (Group B). After 8 wk, PSG and US were repeated in all patients. Platelet deposition was assessed visually and semi-quant. using a platelet accumulation index. Visual anal. showed that seven out of eight patients became neg. for platelet deposition after treatment in Group B, while none changed in Group A. The platelet accumulation index of vessels with platelet deposition was significantly reduced after treatment in Group B (12.4 ± 3.9% vs. 6.0 ± 7.1%, $p < 0.01$), while there was no significant change in the vessels without platelet deposition (2.9 ± 3.0% vs 2.9 ± 4.1%). In Group A, none of the vessels showed any change (8.1 ± 6.4% vs 8.9 ± 7.3%). However, there was no significant reduction of carotid plaque size in either group. Short-term E5510 therapy inhibited platelet deposition in active atherothrombotic lesions, and the combination of PSG and US was useful for evaluating the effectiveness of anti-thrombotic drugs in vivo.
IT **111753-73-2**, E5510
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(E5510, antiplatelet agent effect on platelet deposition in atherothrombotic lesions evaluated by 111In platelet scintigraphy in humans)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

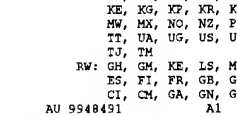


REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

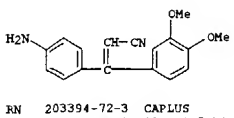
L6 ANSWER 10 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:34743 CAPLUS
DOCUMENT NUMBER: 132:74868
TITLE: Fungal growth inhibitors
INVENTOR(S): Nelson, Richard A.; Bhatia, Mohit B.; Lewis, Craig M.; Zhang, Minghua
PATENT ASSIGNEE(S): Celgro, USA
SOURCE: PCT Int. Appl., 11 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000001387	A1	20000113	WO 1999-US14835	19990630
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
AU 9948491	A1	20000124	AU 1999-48491	19990630
PRIORITY APPLN. INFO.:			US 1998-91367P	P 19980701
			WO 1999-US14835	W 19990630

AB Phosphodiesterase inhibitors are agrochem. antifungal agents. 3,3-Bis-(3-ethoxy-4-methoxyphenyl)propenonitrile is one example.
IT **203394-46-1 203394-59-6 203394-72-3 203394-78-9**
RL: AGR (Agricultural use); BIOL (Biological study); USES (Uses)
(phosphodiesterase inhibitor as agrochem. fungicide)
RN 203394-46-1 CAPLUS
CN 2-Propenenitrile, 3,3-bis(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

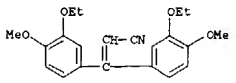


RN 203394-59-6 CAPLUS
CN 2-Propenenitrile, 3-(4-aminophenyl)-3-(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

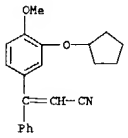


RN 203394-72-3 CAPLUS
CN 2-Propenenitrile, 3,3-bis(3-ethoxy-4-methoxyphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 10 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 203394-78-9 CAPLUS
CN 2-Propenenitrile, 3-[3-(cyclopentyloxy)-4-methoxyphenyl]-3-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

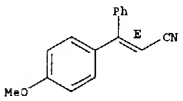
L6 ANSWER 11 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:703200 CAPLUS
DOCUMENT NUMBER: 132:63773
TITLE: New approaches towards the synthesis of alkenes using the Horner-Wadsworth-Emmons (HWE) reaction as the key step
AUTHOR(S): Bodman, Kerstin; Has-Becker, Shenay; Reiser, Oliver
CORPORATE SOURCE: Department of Organic Chemistry, University of Regensburg, Regensburg, D-93053, Germany
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (1999), 144-146, 173-176
CODEN: PSSLEC; ISSN: 1042-6507
PUBLISHER: Gordon & Breach Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:63773

AB Previous work in asym. alkene synthesis revealed that the alkenylation of aldehydes with phosphonates proceeds smoothly at room temperature in the absence of Lewis acid using triethylamine as the base if the reaction is carried out at a pressure of 8 kbar. Based on this protocol a new domino process was developed, combining the HWE reaction with a Heck coupling, thus allowing the one pot synthesis of trisubstituted alkenes.

IT **170879-13-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(stereoselective prepn of alkenes via a high pressure palladium catalyzed combined Horner-Wadsworth-Emmons reaction/Heck reaction of aldehydes with phosphonates and aryl iodides)

RN 170879-13-7 CAPLUS
CN 2-Propenenitrile, 3-(4-methoxyphenyl)-3-phenyl-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



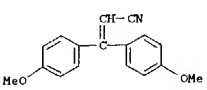
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 12 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:673764 CAPLUS
DOCUMENT NUMBER: 132:23070
TITLE: Azide migration and azide bridging: preparation of metalated acrylonitriles and of dinuclear complexes containing an almost linear eleven-membered C3RhN3RhC3 chain
AUTHOR(S): Laubender, Matthias; Werner, Helmut
CORPORATE SOURCE: Institut fur Anorganische Chemie der Universitat, Wurzburg, D-97074, Germany
SOURCE: Chemistry--A European Journal (1999), 5(10), 2937-2946
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:23070

AB Isoelectronic square-planar azido- and isocyanatorhodium (I) complexes trans-[RhX(:C:C:CRR')(PiPr3)2] (X = N3: 9-12; X = CNO: 13-16) were prepared from the related chloro derivs. trans-[RhCl(:C:C:CRR')(PiPr3)2] by salt metathesis. A single-crystal x-ray diffraction study of 12 (R = Ph, R' = tBu) confirmed an almost linear arrangement of the Rh-C-C-C chain, but a significant bending of the Rh-N-N-N unit. In contrast to the isocyanato complexes 13-16, which are quite inert toward CO, the azido derivs. 9, 11 and 12 react with CO by migratory insertion of the allenylidene ligand into the Rh-N3 bond. While the product obtained from 12 and CO, in which the N3 substituent is linked to the γ-C atom of the C3 chain, is exceedingly stable, the corresponding species with R = R' = aryl are quite labile and rearrange to the metalated acrylonitrile compds. trans-[Rh(C(CN):CRR')(CO)(PiPr3)2] (19, 20) by elimination of N2. The reactions of 19 and 20 (which was crystallog. characterized) with trifluoroacetic acid gave the corresponding acrylonitriles R'RC:CHCN in quant. yields. Treatment of the mononuclear compds. 9-12 with Meerwein's salt [Me3O]BF4 gave dinuclear [(PiPr3)2(R'RC:C:C:)Rh2(μ-1,3-N3)]BF4 (21-24) containing an almost linear eleven-membered C3RhN3RhC3 chain. The x-ray crystal structure anal. of 22 (R = Ph, R' = o-Tol) revealed that the conformations of the two halves of the cation are quite different and that the angle between the two metal-centered planes is 56.5(1)°.

IT **101441-96-7P**, 3,3-Bis(4-methoxyphenyl)propenenitrile
RL: SPN (Synthetic preparation); PREP (Preparation)
(formation by demetalation of rhodium cyanovinyl complex)

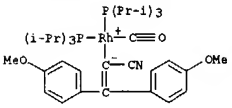
RN 101441-96-7 CAPLUS
CN 2-Propenenitrile, 3,3-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



IT **203869-30-1P**, trans-Carbonyl(1-cyano-2,2-bis(4-methoxyphenyl)vinyl)bis(triisopropylphosphine)rhodium
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, crystal structure and acid-induced demetalation of)

RN 203869-30-1 CAPLUS
CN Rhodium, carbonyl[1-cyano-2,2-bis(4-methoxyphenyl)ethenyl]bis[tris(1-methylethyl)phosphine]-, (SP-4-1)- (9CI) (CA INDEX NAME)

L6 ANSWER 12 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

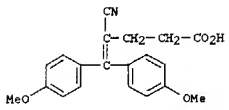


REFERENCE COUNT: 62 THERE ARE 62 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 13 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:619333 CAPLUS
DOCUMENT NUMBER: 131:241350
TITLE: Inhibition of thrombin-induced neuronal cell death by recombinant thrombomodulin and E5510, a synthetic thrombin receptor signaling inhibitor
AUTHOR(S): Sarker, Krishna Pada; Abeyama, Kazuhiro; Nishi, Junichiro; Nakata, Masanori; Tokioka, Takeshi; Nakajima, Toshihiro; Kitajima, Isao; Maruyama, Ikuro
CORPORATE SOURCE: Dep. Laboratory Molecular Medicine, Faculty Medicine, Kagoshima Univ., Kagoshima, 890, Japan
SOURCE: Thrombosis and Haemostasis (1999), 82(3), 1071-1077
CODEN: THHADQ; ISSN: 0340-6245
PUBLISHER: F. K. Schattauer Verlagsgesellschaft mbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Thrombin, a ferine protease generated by the activation of the blood coagulation cascade following vessel injury, converts fibrinogen to fibrin, activates platelets and several coagulation factors, and plays a pivotal role in thrombosis and hemostasis. Thrombin acts as a mitogen and apoptosis inducer in a dose-dependent fashion. The authors have previously shown that thrombin caused proliferation of vascular smooth muscle cells (VSMCs). The authors show that a low concentration of thrombin caused proliferation of mouse neuroblastoma (Neuro-2a) and human neuroblastoma (NB-1) cells, while higher concns. affected cell viability in a time-dependent manner. Similar effects were observed when thrombin receptor agonist peptide (SFLLRNPNDKYEPF, TRAP) was applied. The dying cells showed nuclear condensation and fragmentation, suggesting that cell death occurred by apoptosis. The extent to which thrombin induced cell death was attenuated by recombinant thrombomodulin (rTM), or by a min. functional domain of TM, termed E456. A synthetic compound that inhibits signaling from the thrombin receptor, 4-cyano-5,5-bis (4-methoxyphenyl)-4-pentanoic acid (E5510), and the antioxidant N-acetyl L-Cy (NAC), efficiently prevented thrombin-induced Neuro-2a cell death. Thus, thrombin inhibitors and antioxidant appear to neutralize thrombin toxicity.

IT **111753-73-2**, E5510
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(thrombin-induced neuronal cell death inhibited by recombinant thrombomodulin and E5510, a synthetic thrombin receptor signaling inhibitor)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



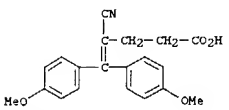
REFERENCE COUNT: 52 THERE ARE 52 CITED REFERENCES AVAILABLE FOR THIS

L6 ANSWER 13 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 14 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:605801 CAPLUS
DOCUMENT NUMBER: 131:222862
TITLE: Satigrel (Eisai)
AUTHOR(S): Clemetson, Kenneth J.
CORPORATE SOURCE: Theodor Kocher Institute, Bern, CH-3012, Switz.
SOURCE: Current Opinion in Anti-Inflammatory and Immunomodulatory Investigational Drugs (1999), 1(3), 277-282
CODEN: COAIFF; ISSN: 1464-8474
PUBLISHER: Current Drugs Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review with 70 refs. Satigrel is a platelet glycoprotein GPIIb/IIIa antagonist and platelet aggregation inhibitor under development by Eisai as a potential antithrombotic. An application was submitted for the approval of satigrel in Japan for the treatment of thrombosis in Dec. 1995. Phase II trials are being conducted in Europe.

IT **111753-73-2**, Satigrel
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(pharmacol. of satigrel)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

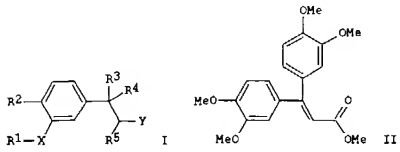


REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 15 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:468066 CAPLUS
DOCUMENT NUMBER: 131:129756
TITLE: Preparation of styrene derivatives as immunotherapeutic agents
INVENTOR(S): Muller, George W.; Shire, Mary
PATENT ASSIGNEE(S): Celgene Corp., USA
SOURCE: U.S., 18 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5929117	A	19990727	US 1997-909201	19970811
CN 1228080	A	19990908	CN 1997-197251	19970811
PT 918746	T	20030829	PT 1997-936479	19970811
EP 1361210	A2	20031112	EP 2003-2806	19970811
EP 1361210	A3	20031119		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, AL				
ES 2197359	T3	20040101	ES 1997-936479	19970811
KR 2000029913	A	20000525	KR 1999-701102	19990210
US 6130226	A	20001010	US 1999-271683	19990318
US 6262101	B1	20010717	US 2000-639757	20000816
US 2001056107	A1	20011227	US 2001-906155	20010716
US 6479554	B2	20021112		
US 2003045726	A1	20030306	US 2002-243927	20020913
US 2004019106	A1	20040129	US 2003-622618	20030717
PRIORITY APPLN. INFO.:			US 1996-695599	B2 19960812
			EP 1997-936479	A3 19970811
			US 1997-909201	A3 19970811
			US 1999-271683	A3 19990318
			US 2000-639757	A3 20000816
			US 2001-906155	A3 20010716
			US 2002-243927	A1 20020913

OTHER SOURCE(S): MARPAT 131:129756
GI

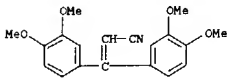


AB Cyano and carboxy derivs. of substituted styrenes, specifically I, are disclosed [wherein Y = COZ, -C.tplbond.N, or lower alkyl; X = O or CnH2n (n = 0-3) and R1 = alkyl, (poly)cycloalkyl, or benzocyclic alkyl; or X = CH and R1 = alkylidene, or (bi)cycloalkylidene; Z = OH, NR6R6, R7, or OR7;

L6 ANSWER 15 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
R6 = H, alkyl; R7 = alkyl, benzyl; R2 = H, NO2, cyano, CF3, CO2H or its Me, Et, or Pr esters, Ac, CONH2, OAc, OH, NH2, alkyl, alkoxy, halo, alkylidenemethyl; R3 = (un)substituted Ph, pyridyl, or cycloalkyl, pyrrolidinyl, imidazolyl, naphthyl, or thienyl; R4 = R5 = H, or R4R5 = bond]. The compds. are inhibitors of tumor necrosis factor α, nuclear factor κB, and phosphodiesterase, and can be used to combat cachexia, endotoxic shock, retrovirus replication, asthma, and inflammatory conditions (no data). Thirty-four preparative and six formulation examples are given, and addnl. example compds. are claimed. A typical embodiment is Me 3,3-bis-(3,4-dimethoxyphenyl)acrylate (II). Wittig-type reaction of tri-Me phosphonoacetate with 3,4,3',4'-tetramethoxybenzophenone in THF in the presence of LiN(SiMe3)2 gave 12% II after flash chromatog.

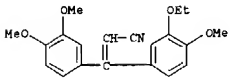
IT **203394-46-1P**, 3,3-Bis-(3,4-dimethoxyphenyl)acrylonitrile **203394-47-2P**, 3-(3,4-Dimethoxyphenyl)-3-(3-ethoxy-4-methoxyphenyl)acrylonitrile **203394-53-0P**, 3-(3-Ethoxy-4-methoxyphenyl)-3-phenylacrylonitrile **203394-55-2P**, 3-(3,4-Dimethoxyphenyl)-3-(3,5-dimethoxyphenyl)acrylonitrile **203394-56-3P**, 3-(3,4-Dimethoxyphenyl)-3-(3-nitrophenyl)acrylonitrile **203394-57-4P**, 3-(3-Aminophenyl)-3-(3,4-dimethoxyphenyl)acrylonitrile **203394-58-5P**, 3-(3,4-Dimethoxyphenyl)-3-(4-nitrophenyl)acrylonitrile **203394-59-6P**, 3-(4-Aminophenyl)-3-(3,4-dimethoxyphenyl)acrylonitrile **203394-60-9P**, 3-(3,4-Dimethoxyphenyl)-3-(4-methylphenyl)acrylonitrile **203394-61-0P**, 3-(4-Biphenylyl)-3-(3,4-dimethoxyphenyl)acrylonitrile **203394-62-1P**, 3-(3,4-Dimethoxyphenyl)-3-(4-fluorophenyl)acrylonitrile **203394-63-2P**, 3-(3,4-Dimethoxyphenyl)-3-(naphth-2-yl)acrylonitrile **203394-64-3P**, 3-(3,4-Dimethoxyphenyl)-3-(3,4-methylenedioxyphenyl)acrylonitrile **203394-70-1P**, 3-(3,4-Diethylphenyl)-3-(3,4-dimethoxyphenyl)acrylonitrile **203394-72-3P**, 3,3-Bis-(3-ethoxy-4-methoxyphenyl)acrylonitrile **203394-75-6P**, 3-(3-Propoxy-4-methoxyphenyl)-3-phenylacrylonitrile **203394-76-7P**, 3,3-Bis-(3-cyclopentoxy-4-methoxyphenyl)acrylonitrile **203394-78-9P**, 3-(3-Cyclopentoxy-4-methoxyphenyl)-3-phenylacrylonitrile **203394-86-9P**, 3-(3,4-Dimethoxyphenyl)-3-phenylacrylonitrile **203395-34-0P**, 3-(3,4-Dimethoxyphenyl)-3-(4-methoxy-3-exo-norbornyloxyphenyl)prop-2-enenitrile **203395-35-1P**, 3-(4-Aminophenyl)-3-(3-ethoxy-4-methoxyphenyl)prop-2-enenitrile
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(target compound; preparation of styrene derivs. as inhibitors of TNFα, NFκB, and phosphodiesterase)

RN 203394-46-1 CAPLUS
CN 2-Propenenitrile, 3,3-bis(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

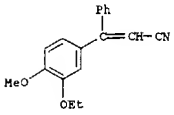


RN 203394-47-2 CAPLUS

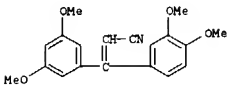
L6 ANSWER 15 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-(3-ethoxy-4-methoxyphenyl)-(9CI) (CA INDEX NAME)



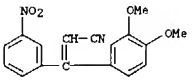
RN 203394-53-0 CAPLUS
CN 2-Propenenitrile, 3-(3-ethoxy-4-methoxyphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



RN 203394-55-2 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-(3,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

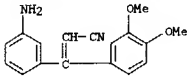


RN 203394-56-3 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

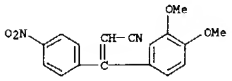


RN 203394-57-4 CAPLUS
CN 2-Propenenitrile, 3-(3-aminophenyl)-3-(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

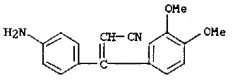
L6 ANSWER 15 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



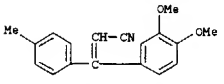
RN 203394-58-5 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



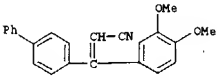
RN 203394-59-6 CAPLUS
CN 2-Propenenitrile, 3-(4-aminophenyl)-3-(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



RN 203394-60-9 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-(4-methylphenyl)- (9CI) (CA INDEX NAME)

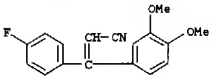


RN 203394-61-0 CAPLUS
CN 2-Propenenitrile, 3-[1,1'-biphenyl]-4-yl-3-(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

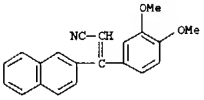


RN 203394-62-1 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-(4-fluorophenyl)- (9CI) (CA INDEX NAME)

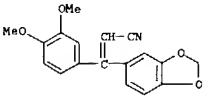
L6 ANSWER 15 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



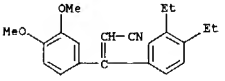
RN 203394-63-2 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)



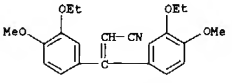
RN 203394-64-3 CAPLUS
CN 2-Propenenitrile, 3-(1,3-benzodioxol-5-yl)-3-(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



RN 203394-70-1 CAPLUS
CN 2-Propenenitrile, 3-(3,4-diethylphenyl)-3-(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

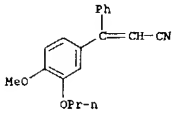


RN 203394-72-3 CAPLUS
CN 2-Propenenitrile, 3,3-bis(3-ethoxy-4-methoxyphenyl)- (9CI) (CA INDEX NAME)

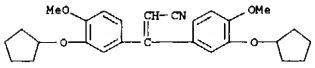


RN 203394-75-6 CAPLUS

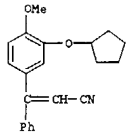
L6 ANSWER 15 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 2-Propenenitrile, 3-(4-methoxy-3-propoxyphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



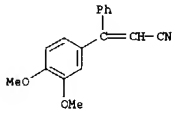
RN 203394-76-7 CAPLUS
CN 2-Propenenitrile, 3,3-bis[3-(cyclopentyloxy)-4-methoxyphenyl]- (9CI) (CA INDEX NAME)



RN 203394-78-9 CAPLUS
CN 2-Propenenitrile, 3-[3-(cyclopentyloxy)-4-methoxyphenyl]-3-phenyl- (9CI) (CA INDEX NAME)



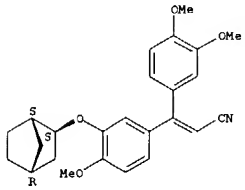
RN 203394-86-9 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



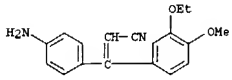
RN 203395-34-0 CAPLUS

L6 ANSWER 15 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 2-Propenenitrile, 3-[3-[(1R,2R,4S)-bicyclo[2.2.1]hept-2-yloxy]-4-methoxyphenyl]-3-(3,4-dimethoxyphenyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

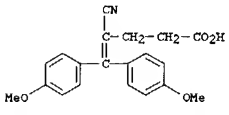


RN 203395-35-1 CAPLUS
CN 2-Propenenitrile, 3-(4-aminophenyl)-3-(3-ethoxy-4-methoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 16 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:360764 CAPLUS
DOCUMENT NUMBER: 131:153337
TITLE: Satigrel; Eisai
AUTHOR(S): Clemetson, Kenneth J.
CORPORATE SOURCE: Theodor Kocher Institute, Berne, CH-3012, Switz.
SOURCE: Current Opinion in Cardiovascular, Pulmonary & Renal Investigational Drugs (1999), 1(1), 93-98
CODEN: CCPRFX; ISSN: 1464-8482
PUBLISHER: Current Drugs Ltd.
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review with 70 refs. Satigrel is a platelet-aggregation inhibitor under development by Eisai as a potential antithrombotic. An NDA was submitted in Japan for the treatment of thrombosis in Dec. 1995 [211508]. Phase II trials are being conducted in Europe [211582].
IT **111753-73-2**, Satigrel
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(pharmacol. of the antithrombotic agent satigrel)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 67 THERE ARE 67 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 17 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:311420 CAPLUS
DOCUMENT NUMBER: 130:329043
TITLE: Use of 1,1-dicyano-2,2-diphenylethene and its derivatives against the UV-induced decomposition of dibenzoylmethane and its derivatives
INVENTOR(S): Scheel, Oliver; Gers-Barlag, Heinrich
PATENT ASSIGNEE(S): Beiersdorf A.-G., Germany
SOURCE: Ger. Offen., 18 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

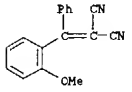
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19748755	A1	19990506	DE 1997-19748755	19971105
PRIORITY APPLN. INFO.:			DE 1997-19748755	19971105

OTHER SOURCE(S): MARPAT 130:329043
AB 1,1-Dicyano-2,2-diphenylethene and its derivs. R1nC6H4(R2mC6H4)C:C(CN)2 (R1, R2 = H, o- or p-Cl-18 alkyl, alkoxy, cycloalkyl, or cycloalkoxy; m, n = 1, 2) are useful in cosmetic and dermatol. sunscreen prepns. to stabilize dibenzoylmethane UV filter compds. against UV-induced photolytic decomposition. Thus, an oil-in-water sunscreen lotion contained glyceryl stearate 3.50, stearic acid 1.80, glycerin 3.00, cetostearyl alc. 0.50, 45% NaOH solution 0.20, octyldodecanol 7.00, dicaprylyl ether 8.00, 2,4,6-trianilino-(p-carbo-2'-ethyl-1'-hexyloxy)-1,3,5-triazine 3.00, 1,1-dicyano-2-phenyl-2-(p-butoxyphenyl)ethene 3.00, 4-(tert-butyl)-4'-methoxydibenzoylmethane 2.00, 2,2-dimethyl-1,3-propanediol diheptanoate 6.00, Carbomer 0.20, preservative, perfume, and H2O to 100.00 weight%.
IT **190316-22-4**
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(use of dicyanodiphenylethene and its derivs. against UV-induced decomposition of dibenzoylmethane derivs.)
RN 190316-22-4 CAPLUS
CN Propanedinitrile, [(4-butoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 18 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:242846 CAPLUS
DOCUMENT NUMBER: 130:358967
TITLE: X-ray diffraction analysis of NLO single crystals: traditional and non-traditional applications
AUTHOR(S): Antipin, Mikhail Yu.; Clark, Ronald D.; Nesterov, Vladimir N.; Lyssenko, Konstantin A.; Timofeeva, Tatiana V.
CORPORATE SOURCE: Department of Physical Sciences, New Mexico Highlands University, Las Vegas, NM, 87701, USA
SOURCE: Proceedings of SPIE-The International Society for Optical Engineering (1998), 3474(Second-Order Organic Nonlinear Optics), 41-52
CODEN: PSISDG; ISSN: 0277-786X
PUBLISHER: SPIE-The International Society for Optical Engineering
DOCUMENT TYPE: Journal
LANGUAGE: English

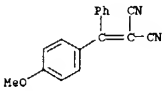
AB The present paper deals with the traditional and some new applications of the single crystal x-ray diffraction anal. of NLO materials. Traditionally, x-ray diffraction was used to prove mol. structure of a compound of interest, to establish crystal space group, packing array and features of the mol. geometry. This approach was used in anal. of a large series of new organic NLO chromophores including substituted dicyanovinylaroms., and some other NLO materials. Most of the compds. studied demonstrate high mol. 2nd-order optical susceptibilities. It was shown for substituted dicyanovinylbenzenes (using mol. mechanics calcns. and crystal packing anal.) what factors are responsible for the centric or acentric crystal structure of a given compound Several new compds. of the series studied exhibit a rather strong 2nd harmonic generation signal in the solid state, in particular, o-fluoro-dicyanovinylbenzene, p-dimethylamino-dicyanovinylbenzene, and 4-(4-methoxyphenyl)-1,1-dicyano-1,3-butadiene, 4-MeO-C6H4-CH=CH-CH=C(CN)2. Mol. and crystal structures of these compds. were studied and analyzed. Another new application of the x-ray diffraction method in the study of NLO compds. is anal. of the electron d. distributions in crystals and direct estimation of some of its characteristics (atomic charges, dipole and higher multipole moments, etc.) responsible for NLO properties directly from the diffraction data. These opportunities of the method were demonstrated in the charge d. study of crystals of DIVA (o-methoxydicyanovinylbenzene) and mNA (m-nitroaniline). Second-order optical susceptibilities were estimated from the diffraction data using a multipole model and are close to the exptl. values.

IT **56822-05-0**
RL: PRP (Properties)
(crystal structure in relation to nonlinear optical properties of)
RN 56822-05-0 CAPLUS
CN Propanedinitrile, [(2-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)



L6 ANSWER 18 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

IT **17212-45-2**
RL: PRP (Properties)
(dipole moments, second order polarizabilities and nonlinear optical properties of)
RN 17212-45-2 CAPLUS
CN Propanedinitrile, [(4-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

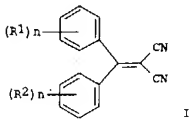


REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 19 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:70352 CAPLUS
DOCUMENT NUMBER: 130:129768
TITLE: Sunscreens comprising dicyanodiphenylethylene derivatives
INVENTOR(S): Bringhen, Alain; Gonzenbach, Hans Ulrich; Pochon, Magali
PATENT ASSIGNEE(S): F. Hoffmann-La Roche Ag, Switz.
SOURCE: Eur. Pat. Appl., 13 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 891766	A1	19990120	EP 1998-112954	19980713
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CA 2241645	AA	19990114	CA 1998-2241645	19980624
AU 9873963	A1	19990121	AU 1998-73963	19980630
AU 735151	B2	20010705		
NO 9803112	A	19990115	NO 1998-3112	19980706
US 6048516	A	20000411	US 1998-113863	19980710
BR 9802481	A	20000208	BR 1998-2481	19980713
JP 11071254	A2	19990316	JP 1998-198345	19980714
CN 1214239	A	19990421	CN 1998-115991	19980714
PRIORITY APPLN. INFO.:			EP 1997-111938 A	19970714

OTHER SOURCE(S): MARPAT 130:129768
GI

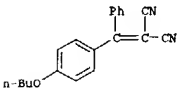


I

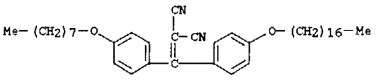
AB A photostabilized dibenzoylmethane type UV-A screening agent stabilized by at least one compound of I (R1 and R2 are equal or different and represent linear or branched alkyl or alkoxy radicals with 1 to 18 C atoms, or one of R1 and R2 is a hydrogen atom and n is 1 or 2) are claimed. Compds. of I were prepared by mixing 40 mmoles of the adequate ketimine with 40 mmoles of malonitrile at room temperature The photostabilization effect of Parsol-1789 brought by 1% 1,1,-dicyano-2-(4-butoxyphenyl)-2-phenylethylene (II) is shown. An oil in water emulsion contained Bu methoxydibenzoylmethane 2, II 1, glycerol monomyristate 4, PVP-eicosen copolymer 2, cetyl alc. 2, caprylic/capric triglyceride 10, butylhydroxytoluene 0.1, preservatives 0.6, Amphisol K 2, propylene glycol 10, disodium EDTA 0.1, Carbomer 981 10, and water 100%.

IT **190316-22-4 219901-72-1**
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

L6 ANSWER 19 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(sunscreens comprising dicyanodiphenylethylene derivs.)
RN 190316-22-4 CAPLUS
CN Propanedinitrile, [(4-butoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)



RN 219901-72-1 CAPLUS
CN Propanedinitrile, [[4-(heptadecyloxy)phenyl][4-(octyloxy)phenyl]methylene]- (9CI) (CA INDEX NAME)

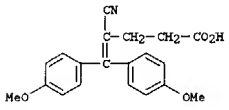


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 20 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1999:26506 CAPLUS
DOCUMENT NUMBER: 130:204885
TITLE: A randomized, placebo-controlled, crossover study of E5510 and aspirin in healthy volunteers
AUTHOR(S): Reilly, Muredach P.; Moran, Niamh; Meagher, Emma; Delanty, Norman; Cucchiara, Andrew E.; Lawson, John A.; Catella-Lawson, Francesca
CORPORATE SOURCE: The Division of Cardiology, University of Pennsylvania, School of Medicine, Philadelphia, PA, USA
SOURCE: Journal of Cardiovascular Pharmacology (1999), 33(1), 12-18
CODEN: JCPCDT; ISSN: 0160-2446
PUBLISHER: Lippincott Williams & Wilkins
DOCUMENT TYPE: Journal
LANGUAGE: English

AB E5510 is a novel compound that has multiple platelet-inhibitory effects in in vitro studies. The in vivo pharmacodynamic effects of maximal antiplatelet doses of E5510 (20 mg) were compared with those of 300 mg aspirin in a placebo-controlled, triple crossover trial in healthy volunteers. Collagen-induced platelet aggregation and serum thromboxane B2 (TxB2) were similarly inhibited by both compds. in the 1st 12 h but showed recovery at 24 h in the E5510-treated group only. Thrombin- and U46619-induced platelet aggregation, as well as basal and PGE2-stimulated platelet cAMP levels were unchanged after ingestion of either agent. E5510 and aspirin reduced systemic thromboxane formation without affecting prostacyclin biosynthesis. Neither E5510 nor aspirin inhibited the excretion of 8-epi PGF2α and 5,6-dihydroxyeicosatrienoic acid, 2 indexes of cyclooxygenase-independent arachidonate metabolism In conclusion:
(a) E5510 in vivo most likely induces a reversible inhibition of cyclooxygenase, without affecting thromboxane synthetase, phosphodiesterase, thrombin, or thromboxane receptor-mediated signaling; (b) single doses of aspirin or E5510 affect thromboxane/prostacyclin profiles favorably, supporting their use in acute coronary syndromes. This study outlines a comprehensive and minimally invasive approach for the assessment of the in vivo mechanism of action of novel antiplatelet agents.

IT **111753-73-2**, E 5510
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(platelet function of humans response to aspirin vs.)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



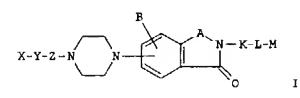
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS

L6 ANSWER 20 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

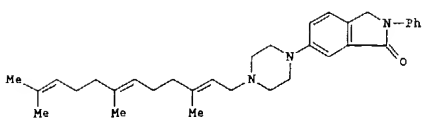
L6 ANSWER 21 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:793126 CAPLUS
DOCUMENT NUMBER: 130:52434
TITLE: Preparation of nitrogenous heterocyclic compounds as hyperlipemia remedies
INVENTOR(S): Ohkura, Naoto; Tsuruoka, Takashi; Usui, Takayuki; Hiraiwa, Yukiko; Matsushima, Tetsuya; Shiotani, Masaharu; Niizato, Tetsutaro; Nakatani, Yuuko; Suzuki, Shigeki; Kuroda, Chidsuko; Katano, Kiyoaki
PATENT ASSIGNEE(S): Meiji Seika Kaisha, Ltd., Japan; et al.
SOURCE: PCT Int. Appl., 194 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9854135	A1	19981203	WO 1998-JP2411	19980601
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9875482	A1	19981230	AU 1998-75482	19980601
EP 999208	A1	20000510	EP 1998-923066	19980601
R: DE, ES, FR, GB, IT				
US 6417362	B1	20020709	US 1999-424708	19991130
US 2002156276	A1	20021024	US 2002-127491	20020423
US 6583144	B2	20030624		
PRIORITY APPLN. INFO.:			JP 1997-141410 A	19970530
			WO 1998-JP2411 W	19980601
			US 1999-424708 A3	19991130

OTHER SOURCE(S): MARPAT 130:52434
GI



I

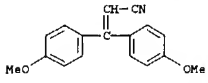


II

L6 ANSWER 21 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

AB The title compds. [I; A = CR1R2(CH2)i; (wherein R1 and R2 each represents hydrogen or alkyl, i = 0-1), CH:CH, OCH2, or S(O)jCH2 (wherein j = 0-2); B = hydrogen or halogen; X = CR3R4R5, NR6R7, (CH2CH:C(CH3)CH2)pCH2CH:C(CH3)2, alkyl, cycloalkyl, Ph, cinnamyl, or heteroaryl; Y = (CH2)q, CH:CH, NR8, oxygen, or a bond; Z = carbonyl or a bond; K = alkylene or a bond; L = CH:CH or a bond; and M = hydrogen, alkyl, cycloalkyl, Ph, heterocycle, biphenyl, or diphenymethyl; p = 0-2; q = 1-6; R3-R5 = hydrogen, phenyl; R6-R7 = hydrogen, Ph, benzyl; R8 = hydrogen, C1-6 alkyl] are prepared I inhibit the biosynthesis of triglycerides in the liver and also inhibit the secretion of lipoproteins containing apolipoprotein B from the liver. I are hence useful for the prevention/treatment of hyperlipemia (especially hyper-VLDL-emia) and diseases caused thereby, such as arteriosclerotic diseases, e.g., myocardial infarct, and pancreatitis. Thus, title compound (II) was prepared by multi-step reactions and showed 56% and 90% inhibitory activity for apolipoprotein B and triglycerides. A formulation containing I was also presented.

IT **101441-96-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of nitrogenous heterocyclic compds. as hyperlipemia remedies)
RN 101441-96-7 CAPLUS
CN 2-Propenenitrile, 3,3-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 22 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:603186 CAPLUS
DOCUMENT NUMBER: 129:193536
TITLE: Methods and compositions using retinoids for preventing and treating chronological aging in human skin
INVENTOR(S): Varani, James; Fisher, Gary J.; Voorhees, John J.; Kang, Sewon
PATENT ASSIGNEE(S): The Regents of the University of Michigan, USA
SOURCE: PCT Int. Appl., 46 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9836742	A1	19980827	WO 1998-US3743	19980223
W: AU, BB, BG, BR, CA, CN, CU, CZ, EE, HU, ID, IL, IS, JP, KR, LC, LT, LV, MK, MN, MW, MX, NO, NZ, PL, RO, SG, SK, SL, TR, TT, UA, UG, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9865374	A1	19980909	AU 1998-65374	19980223
AU 737376	B2	20010816		
BR 9807854	A	20000222	BR 1998-7854	19980223
EP 1005333	A1	20000607	EP 1998-911417	19980223
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 2002515898	T2	20020528	JP 1998-537021	19980223
US 2001053347	A1	20011220	US 1998-28435	19980224
US 6630516	B2	20031007		
US 2004034098	A1	20040219	US 2003-458355	20030610

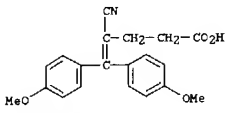
PRIORITY APPLN. INFO.: US 1997-40594P P 19970225
US 1997-42976P P 19970407
US 1998-73214P P 19980130
WO 1998-US3743 W 19980223
US 1998-28435 A3 19980224

AB The deleterious effects of the passage of time on human skin (i.e., chronol. aging of human skin) can be prevented and treated with the topical application of a retinoid, preferably retinol. We have found that some of the same pathways (namely the stress-activated pathways, SAPs) activated in photoaging of human skin (i.e., sun-induced premature skin aging) are similarly elevated in the skin of elderly people. We have also found that other pathways (namely the mitogen-activated ERK pathway) is depressed in the same skin. Treatment of chronol.-aged skin with a retinoid both inhibits degradation of dermal collagen and promotes procollagen synthesis. Biopsied sections from skin of elderly (80+ years old) show that a single treatment can increase epidermal thickness, improve the dermal collagen d., and promote the formation of rete pegs and dermal papillae, and can decrease the amount of c-Jun and increase the amts. of Types I and III procollagen. Such benefits are also helpful in preventing bruising, tearing, and ulceration of elderly skin.

IT **111753-73-2**, E5510

L6 ANSWER 22 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(retinoids for preventing and treating chronol. aging in human skin)

RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



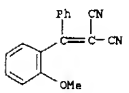
REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 23 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:532126 CAPLUS
DOCUMENT NUMBER: 129:244724
TITLE: Molecular Crystal Structures and Nonlinear Optical Properties in the Series of Dicyanovinylbenzene and Its Derivatives
AUTHOR(S): Antipin, Mikhail Yu.; Timofeeva, Tatiana V.; Clark, Ronald D.; Nesterov, Vladimir N.; Sanghadasa, Mohan; Barr, Thomas A.; Penn, Benjamin; Romero, Leonard; Romero, Melvin
CORPORATE SOURCE: Department of Physical Sciences, New Mexico Highlands University, Las Vegas, NM, 87701, USA
SOURCE: Journal of Physical Chemistry A (1998), 102(37), 7222-7232
CODEN: JPCAFH; ISSN: 1089-5639
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB X-ray single-crystal structures, mol. mechanics (MM) calcns. of the optimal mol. dimers, and calcns. of the static second-order polarizabilities (β) were performed for a large series of methoxy- and dimethylamino-substituted derivs. of dicyanovinylbenzene and some of its analogs having large values for the mol. nonlinear optical susceptibilities. X-ray structural anal. has been performed for 3,4-dimethoxy- and 3,4,5-trimethoxy-1-(2,2-dicyanovinyl)benzenes (I, II), 4-(dimethylamino)-1-(2,2-dicyanovinyl)benzene (III), 1,1-dicyano-2-phenyl-2-(2-methoxyphenyl)ethene (2-MeO-C6H4-C(C6H5):C(CN)2) (IV), and 4-(4-methoxyphenyl)-1,1-dicyano-1,3-butadiene (4-MeO-C6H4-CH:CH-CH:C(CN)2) (V). Crystal packing anal. and energetic MM calcns. revealed the factors responsible for the formation of the centrosym. crystals. Compds. III and V were found to form acentric crystal structures (space groups P21 and Pc, resp.) and, therefore, are capable of the second-harmonic generation (SHG) in the solid state. Qual. data have demonstrated that compound V is rather active in SHG in the powder state (using Nd:YAG laser with λ = 1064 nm) that may be important for its application. On the contrary, the powder of III is not active in SHG despite the "optimal" crystal packing that might be related to the strong absorption of the second harmonic light at λ = 532 nm, but this compound gives strong SHG signal using the laser light with λ = 1907 nm. Anal. of the influence of the different substituents in the aromatic ring on the calculated β values in the series of the compds. studied was made.

IT **56822-05-0**, 1,1-Dicyano-2-phenyl-2-(2-methoxyphenyl)ethene
RL: PRP (Properties)
(crystallog. and calculated values for second-order polarizabilities of a large series of methoxy- and dimethylamino-substituted derivs. of dicyanovinylbenzene and some of its analogs)

RN 56822-05-0 CAPLUS
CN Propanedinitrile, [(2-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

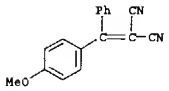
L6 ANSWER 23 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L6 ANSWER 24 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:441612 CAPLUS
DOCUMENT NUMBER: 129:148730
TITLE: Molecular design and nonlinear optical properties in the series of substituted dicyanovinylaromatics
AUTHOR(S): Antipin, Mikhael Yu.; Clark, Ronald D.; Nesterov, Vladimir N.; Sanghadasa, Mohan; Timofeeva, Tatiana V.; Lyssenko, Konstantin A.
CORPORATE SOURCE: Department of Physical Sciences, New Mexico Highlands University, Las Vegas, NM, 87701, USA
SOURCE: Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1998), 313, 85-94
CODEN: MCLCE9; ISSN: 1058-725X
PUBLISHER: Gordon & Breach Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: English

AB X-ray single-crystal study and mol.-mechanics and quantum-chemical calcns. of the static nonlinear optical (NLO) polarizabilities (β) were performed for a large series of dicyanovinylarom. derivs. in order to draw conclusions about the relationship between their mol. geometry, crystal structure and NLO properties. EFISH measurements of the β values in solns. were made for some compds. studied, and good correlation was found between the calculated and exptl. values. X-ray data and optimal mol.-associate calcns. revealed the factors responsible for formation of centric/acentric crystal structures. This approach might be useful for prediction of possible crystal structures for simple organic chromophores. Only 3 acentric crystal structures were found in the series studied, and in agreement with their mol., electronic and crystal-packing characteristics, all were active in 2nd-harmonic generation (SHG) in the solid state. High-resolution low-temperature (153 K) multipole x-ray diffraction anal. of the electron-d. distribution was performed for the known NLO crystal of (dicyanovinyl)anisole, and these data were used to estimate the mol. dipole moment and β values directly from the x-ray diffraction data.

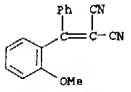
IT **17212-45-2**, Propanedinitrile, [(4-methoxyphenyl)phenylmethylene]- **56822-05-0**, Propanedinitrile, [(2-methoxyphenyl)phenylmethylene]-
RL: PRP (Properties)
(mol. design and nonlinear optical properties in series of substituted dicyanovinyl aromatic compds.)

RN 17212-45-2 CAPLUS
CN Propanedinitrile, [(4-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)



RN 56822-05-0 CAPLUS
CN Propanedinitrile, [(2-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX

L6 ANSWER 24 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 25 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:206305 CAPLUS
DOCUMENT NUMBER: 129:12343
TITLE: Clomiphene analogs with activity in vitro and in vivo against human breast cancer cells
AUTHOR(S): Baumann, R. Jeffrey; Bush, Tammy L.; Cross-Doersen, Doreen E.; Cashman, Elizabeth A.; Wright, Paul S.; Zwolshen, John H.; Davis, Gregory F.; Matthews, Donald P.; Bender, David M.; Bitonti, Alan J.
CORPORATE SOURCE: ONCOLOGY, HOECHST MARION ROUSSEL, BRIDGEWATER, NJ, 08807, USA
SOURCE: Biochemical Pharmacology (1998), 55(6), 841-851
CODEN: BCPCA6; ISSN: 0006-2952
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Six hundred triphenylethylenes were assayed for antiproliferative activity against MCF-7, LY2, and MDA-MB-231 breast cancer cells using sulforhodamine B dye to measure proliferation. Here we report on just 63 of the compds., mostly clomiphene analogs, with substitutions on the α' or β ring, at the vinyl position or in the side chain, of which 23 were active, as defined by antiproliferation IC50 values ≤1 μM. Activity profiles showed that 23 and 11 analogs were active toward MCF-7 and LY2, resp., but none were active against MDA-MB-231. The IC50 values of tamoxifen were 2.0 μM against MCF-7 and 7.5 μM against LY2 and MDA-MB-231. Estradiol reversed antiproliferative activities of several E isomers but not their Z isomer counterparts. Clomiphene side chain analogs 46 [(E)-1-butanamine, 4-[4-(2-chloro-1,2-diphenylethenyl) phenoxy]-N,N-diethyl-dihydrogen citrate (MDL 103,323)] and 57 [(E)-N-[p-(2-chloro-1,2-diphenylvinyl) phenyl]-N,N-diethylethylenediamine dihydrogen citrate (MDL 101,986)] were 4- to 5-fold more effective than tamoxifen. Methylene addns. up to (-CH2-)12 in the clomiphene side chain showed that analog 46 [(-CH2-)4 side chain] had maximal antiproliferative activity, binding affinity, and inhibition of transcription of an estrogen response element luciferase construct in transfected MCF-7 cells. I.p. administration of 46 or 57 inhibited progression of MCF-7 breast tumor xenografts in nude mice with ED50 values of <0.02 mg/mouse/day. Both analogs may hold promise for treating ER pos. breast cancer and are of interest for further development.

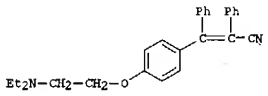
IT **207562-98-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(triphenylethylene clomiphene analogs and their activity in vitro and in vivo against human breast cancer cells)

RN 207562-98-9 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl]phenylmeth ylene]-, 2-hydroxy-1,2,3-propanetricarboxylate (1:1) (9CI) (CA INDEX NAME)

CM 1

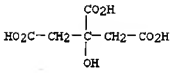
CRN 207562-97-8
CMF C27 H28 N2 O

L6 ANSWER 25 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



CM 2

CRN 77-92-9
CMF C6 H8 O7



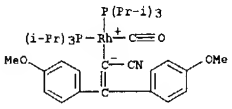
REFERENCE COUNT: 46 THERE ARE 46 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 26 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:150902 CAPLUS
DOCUMENT NUMBER: 128:204982
TITLE: Unprecedented C-N coupling following migration of an azido ligand to a C:C:CRR' unit
AUTHOR(S): Laubender, Matthias; Werner, Helmut
CORPORATE SOURCE: Dept. Chem. M. Laubender, Inst. fur Anorganische Chemie der Univ. Am Hubland, Wurzburg, D-97074, Germany
SOURCE: Angewandte Chemie, International Edition (1998), 37(1/2), 150-152
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:204982

AB Complexes trans-[RhN3(PiPr3)2(C:C:CRR')] (R = Ph, p-C6H4OMe; R' = Ph, tBu, p-C6H4OMe) were prepared in practically quant. yields by treating complexes trans-[RhCl(PiPr3)2(C:C:CRR')] (same R, same R') with excess NaN3 in a 1:1 mixture of acetone and THF at room temperature. CO was then passed through a toluene solution of the products at -60° for 30s. For R = Ph and R' = tBu trans-(Rh(CO)(PiPr3)2C.tplbond.CCN3PhtBu] was obtained in 90% yield. For R = R' = Ph and R = R' = p-C6H4OMe the complexes trans-[RhCO(PiPr3)2C(CN):CRR'] were obtained in 90% yield. The crystal structures of trans-[RhN3(PiPr3)2C:C:CPhtBu] (space group P.hivin.1, Z = 2, R1 = 0.0399, wR2 = 0.0839) and trans-[Rh(CO)(PiPr3)2C(CN):C(p-C6H4OMe)2] (space group P21/c, Z = 4, R1 = 0.0340, wR2 = 0.0703) were determined

IT **203869-30-1P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (crystal structure; carbon-nitrogen coupling reaction following migration of an azido ligand)

RN 203869-30-1 CAPLUS
CN Rhodium, carbonyl[1-cyano-2,2-bis(4-methoxyphenyl)ethenyl]bis[tris(1-methylethyl)phosphine]-, (SP-4-1)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 27 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:126232 CAPLUS
DOCUMENT NUMBER: 128:192444
TITLE: Novel styrene derivatives and analogs useful as immunotherapeutic agents, and their use in the reduction of cytokine levels
INVENTOR(S): Muller, George W.; Shire, Mary
PATENT ASSIGNEE(S): Celgene Corporation, USA; Muller, George W.; Shire, Mary
SOURCE: PCT Int. Appl., 56 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9806692	A1	19980219	WO 1997-US14098	19970811
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9739138	A1	19980306	AU 1997-39138	19970811
AU 729247	B2	20010125		
EP 918746	A1	19990602	EP 1997-936479	19970811
EP 918746	B1	20030409		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
CN 1228080	A	19990908	CN 1997-197251	19970811
JP 2000516616	T2	20001212	JP 1998-509944	19970811
NZ 334148	A	20011221	NZ 1997-334148	19970811
RU 2188819	C2	20020910	RU 1999-104523	19970811
AT 236872	E	20030415	AT 1997-936479	19970811
PT 918746	T	20030829	PT 1997-936479	19970811
EP 1361210	A2	20031112	EP 2003-2806	19970811
EP 1361210	A3	20031119		
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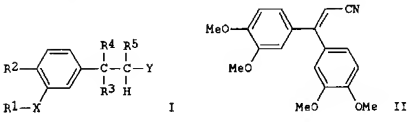
ES 2197359	T3	20040101	ES 1997-936479	19970811
FI 9900180	A	19990308	FI 1999-180	19990201
KR 2000029913	A	20000525	KR 1999-701102	19990210
HK 1021814	A1	20031205	HK 1999-105649	19991202
US 2001056107	A1	20011227	US 2001-906155	20010716
US 6479554	B2	20021112		
PRIORITY APPLN. INFO.:			US 1996-695599 A	19960812
			EP 1997-936479 A3	19970811
			WO 1997-US14098 W	19970811
			US 2000-639757 A3	20000816

OTHER SOURCE(S): MARPAT 128:192444
GI

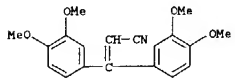
L6 ANSWER 27 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



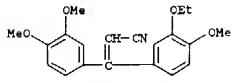
AB Cyano and carboxy derivs. of substituted styrenes I are inhibitors of tumor necrosis factor α, nuclear factor κB, and phosphodiesterase, and can be used to combat cachexia, endotoxic shock, retrovirus replication, asthma, and inflammatory conditions [wherein Y = CO2, -C.tplbond.N, or lower alkyl; X = O or CnH2n (n = 0-3) and R1 = alkyl, (poly)cycloalkyl, or benzocyclic alkyl; or X = CH and R1 = alkylidene, or (bi)cycloalkylidene; Z = OH, NR6R6, R7, or OR7; R6 = H, alkyl; R7 = alkyl, benzyl; R2 = H, NO2, cyano, CF3, CO2H or its Me, Et, or Pr esters, Ac, CONH2, OAc, OH, NH2, alkyl, alkoxy, halo, alkylidenemethyl; R3 = (un)substituted Ph, pyridyl, or cycloalkyl, pyrrolidinyl, imidazolyl, naphthyl, or thienyl; R4 = R5 = H, or R4R5 = bond]. Thirty preparative and six formulation examples are given, and a large number of addnl. example compds. are claimed. A typical embodiment is 3,3-bis-(3,4-dimethoxyphenyl)acrylonitrile (II). Friedel-Crafts acylation of veratrole with 3,4-dimethoxybenzoyl chloride gave 66% 3,4,3',4'-tetramethoxybenzophenone, which underwent Wittig reaction with di-Et cyanomethylphosphonate using NaH in THF to give II.

IT **203394-46-1P**, 3,3-Bis(3,4-dimethoxyphenyl)acrylonitrile **203394-47-2P**, 3-(3,4-Dimethoxyphenyl)-3-(3-ethoxy-4-methoxyphenyl)acrylonitrile **203394-53-0P**, 3-(3-Ethoxy-4-methoxyphenyl)-3-phenylacrylonitrile **203394-55-2P**, 3-(3,4-Dimethoxyphenyl)-3-(3,5-dimethoxyphenyl)acrylonitrile **203394-56-3P**, 3-(3,4-Dimethoxyphenyl)-3-(3-nitrophenyl)acrylonitrile **203394-57-4P**, 3-(3-Aminophenyl)-3-(3,4-dimethoxyphenyl)acrylonitrile **203394-58-5P**, 3-(3,4-Dimethoxyphenyl)-3-(4-nitrophenyl)acrylonitrile **203394-59-6P**, 3-(4-Aminophenyl)-3-(3,4-dimethoxyphenyl)acrylonitrile **203394-60-9P**, 3-(3,4-Dimethoxyphenyl)-3-(4-methylphenyl)acrylonitrile **203394-61-0P**, 3-(4-Biphenylyl)-3-(3,4-dimethoxyphenyl)acrylonitrile **203394-62-1P**, 3-(3,4-Dimethoxyphenyl)-3-(4-fluorophenyl)acrylonitrile **203394-63-2P**, 3-(3,4-Dimethoxyphenyl)-3-(naphth-2-yl)acrylonitrile **203394-64-3P**, 3-(3,4-Dimethoxyphenyl)-3-(3,4-methylenedioxyphenyl)acrylonitrile **203394-70-1P**, 3-(3,4-Diethylphenyl)-3-(3,4-dimethoxyphenyl)acrylonitrile **203394-72-3P**, 3,3-Bis(3-ethoxy-4-methoxyphenyl)acrylonitrile **203394-75-6P**, 3-(3-Propoxy-4-methoxyphenyl)-3-phenylacrylonitrile **203394-76-7P**, 3,3-Bis(3-cyclopentoxy-4-methoxyphenyl)acrylonitrile **203394-78-9P**, 3-(3-Cyclopentoxy-4-methoxyphenyl)-3-phenylacrylonitrile **203394-86-9P**, 3-(3,4-Dimethoxyphenyl)-3-phenylacrylonitrile **203395-13-5P**, 3-(3,4-Dimethoxyphenyl)-3-[3-(cyclopentylidenemethyl)-4-methoxyphenyl]prop-2-enenitrile **203395-14-6P**, 3-[3-(Cyclopentylidenemethyl)-4-methoxyphenyl]-3-phenylprop-2-enenitrile **203395-20-4P**, 3,3-Bis-[3-(cyclopentylidenemethyl)-4-methoxyphenyl]prop-2-enenitrile **203395-34-0P**, 3-(3,4-Dimethoxyphenyl)-3-[4-methoxy-3-(exo-norbornyloxy)phenyl]prop-2-enenitrile **203395-35-1P**, 3-(4-Aminophenyl)-3-(3-ethoxy-4-methoxyphenyl)prop-2-enenitrile
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of diarylacrylonitriles and analogs as immunotherapeutic agents)

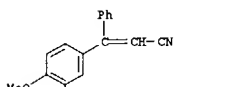
RN 203394-46-1 CAPLUS
CN 2-Propenenitrile, 3,3-bis(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



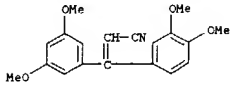
RN 203394-47-2 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-(3-ethoxy-4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 203394-53-0 CAPLUS
CN 2-Propenenitrile, 3-(3-ethoxy-4-methoxyphenyl)-3-phenyl- (9CI) (CA INDEX NAME)

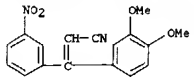


RN 203394-55-2 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-(3,5-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

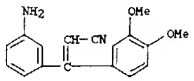


RN 203394-56-3 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

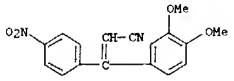
L6 ANSWER 27 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



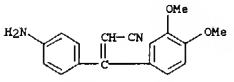
RN 203394-57-4 CAPLUS
CN 2-Propenenitrile, 3-(3-aminophenyl)-3-(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



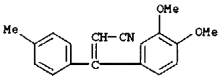
RN 203394-58-5 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-(4-nitrophenyl)- (9CI) (CA INDEX NAME)



RN 203394-59-6 CAPLUS
CN 2-Propenenitrile, 3-(4-aminophenyl)-3-(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

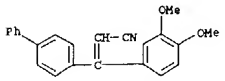


RN 203394-60-9 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-(4-methylphenyl)- (9CI) (CA INDEX NAME)

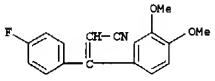


RN 203394-61-0 CAPLUS

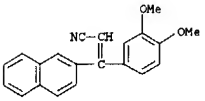
L6 ANSWER 27 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 2-Propenenitrile, 3-[1,1'-biphenyl]-4-yl-3-(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



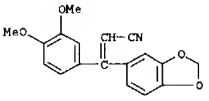
RN 203394-62-1 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



RN 203394-63-2 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-(2-naphthalenyl)- (9CI) (CA INDEX NAME)

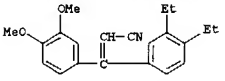


RN 203394-64-3 CAPLUS
CN 2-Propenenitrile, 3-(1,3-benzodioxol-5-yl)-3-(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

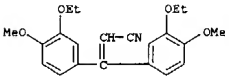


RN 203394-70-1 CAPLUS
CN 2-Propenenitrile, 3-(3,4-diethylphenyl)-3-(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)

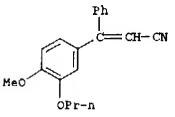
L6 ANSWER 27 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



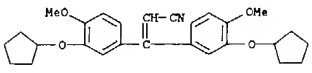
RN 203394-72-3 CAPLUS
CN 2-Propenenitrile, 3,3-bis(3-ethoxy-4-methoxyphenyl)- (9CI) (CA INDEX NAME)



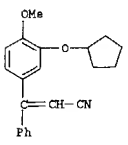
RN 203394-75-6 CAPLUS
CN 2-Propenenitrile, 3-(4-methoxy-3-propoxyphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



RN 203394-76-7 CAPLUS
CN 2-Propenenitrile, 3,3-bis[3-(cyclopentyloxy)-4-methoxyphenyl]- (9CI) (CA INDEX NAME)

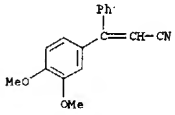


RN 203394-78-9 CAPLUS
CN 2-Propenenitrile, 3-[3-(cyclopentyloxy)-4-methoxyphenyl]-3-phenyl- (9CI) (CA INDEX NAME)

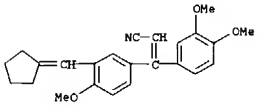


L6 ANSWER 27 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

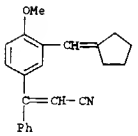
RN 203394-86-9 CAPLUS
CN 2-Propenenitrile, 3-(3,4-dimethoxyphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



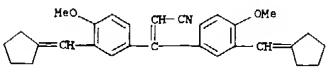
RN 203395-13-5 CAPLUS
CN 2-Propenenitrile, 3-[3-(cyclopentylidenemethyl)-4-methoxyphenyl]-3-(3,4-dimethoxyphenyl)- (9CI) (CA INDEX NAME)



RN 203395-14-6 CAPLUS
CN 2-Propenenitrile, 3-[3-(cyclopentylidenemethyl)-4-methoxyphenyl]-3-phenyl- (9CI) (CA INDEX NAME)

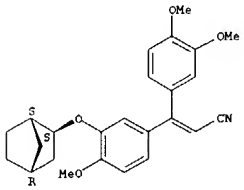


RN 203395-20-4 CAPLUS
CN 2-Propenenitrile, 3,3-bis[3-(cyclopentylidenemethyl)-4-methoxyphenyl]- (9CI) (CA INDEX NAME)

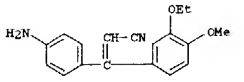


RN 203395-34-0 CAPLUS
CN 2-Propenenitrile, 3-[3-[(1R,2R,4S)-bicyclo[2.2.1]hept-2-yloxy]-4-methoxyphenyl]-3-(3,4-dimethoxyphenyl)-, rel- (9CI) (CA INDEX NAME)

L6 ANSWER 27 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
Relative stereochemistry.
Double bond geometry unknown.

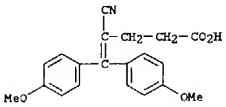


RN 203395-35-1 CAPLUS
CN 2-Propenenitrile, 3-(4-aminophenyl)-3-(3-ethoxy-4-methoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 11 THERE ARE 11 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

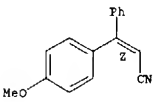
L6 ANSWER 28 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:70556 CAPLUS
DOCUMENT NUMBER: 128:200766
TITLE: Satigrel, a new antiplatelet agent, inhibits platelet accumulation in prosthetic arterial grafts
AUTHOR(S): Esato, Kensuke; Kubo, Yoshihiko; Yasuda, Keishu; Shigematsu, Hiroshi; Iwai, Takehisa; Ishimaru, Shin; Uchida, Hatsuzo; Ishii, Katsumi
CORPORATE SOURCE: First Department of Surgery, Yamaguchi University School of Medicine, Yamaguchi, 755, Japan
SOURCE: American Journal of Surgery (1998), 175(1), 56-60
CODEN: AJSUAB; ISSN: 0002-9610
PUBLISHER: Excerpta Medica, Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The effect of satigrel was studied on the accumulation of indium-labeled platelets in knitted Dacron grafts inserted proximal to the femoral artery. Patients with arteriosclerosis obliterans receiving grafts were treated with satigrel (2 mg twice daily, orally, for 31 days), and others were enrolled as untreated controls. Scintigraphy was performed in postoperative weeks 2 and 4, and the ratio of the scintillation count of the graft to that of the native artery was calculated to assess platelet accumulation. In both weeks 2 and 4, the ratio was smaller in the satigrel-treated group than in the control group for the whole graft, the proximal anastomosis, and the distal anastomosis. Thus, satigrel inhibited platelet accumulation in vascular grafts and may be useful for preventing postoperative graft occlusion.
IT **111753-73-2**, Satigrel
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(platelet accumulation in human prosthetic arterial grafts inhibition by)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

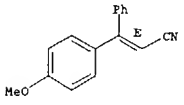
L6 ANSWER 29 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:687538 CAPLUS
DOCUMENT NUMBER: 128:13115
TITLE: Stereospecific preparation of (E)- and (Z)-3,3-diarylacrylonitriles by Heck reaction
AUTHOR(S): Moreno-Manas, Marcial; Pleixats, Roser; Roglans, Anna
CORPORATE SOURCE: Department Chemistry, Universitat Autonoma Barcelona, Barcelona, E-08193, Spain
SOURCE: Synlett (1997), (10), 1157-1158
CODEN: SYNLES; ISSN: 0936-5214
PUBLISHER: Thieme
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:13115
AB (E)- and (Z)-3,3-diarylacrylonitriles are obtained in highly diastereoselective Pd-catalyzed Heck reactions of (E)-cinnamonitriles and aryl iodides under Jeffery conditions.
IT **170879-10-4P 170879-13-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of diarylacrylonitriles by stereoselective Heck reaction)
RN 170879-10-4 CAPLUS
CN 2-Propenenitrile, 3-(4-methoxyphenyl)-3-phenyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 170879-13-7 CAPLUS
CN 2-Propenenitrile, 3-(4-methoxyphenyl)-3-phenyl-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



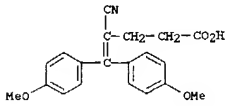
L6 ANSWER 30 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:499085 CAPLUS
DOCUMENT NUMBER: 127:180935
TITLE: Inhibition of skin photoaging by inhibitors of matrix metalloproteinase production
INVENTOR(S): Voorhees, John J.; Fisher, Gary J.
PATENT ASSIGNEE(S): University of Michigan, USA
SOURCE: PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9725969	A1	19970724	WO 1997-US791	19970117
W: AU, BB, BR, BY, CA, CN, CZ, EE, GE, HU, IS, JP, KP, KR, LT, MK, MX, NO, NZ, PL, RO, RU, SG, SI, SK, TR, UA				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5837224	A	19981117	US 1996-588771	19960119
CA 2241981	AA	19970724	CA 1997-2241981	19970117
CA 2241981	C	20020319		
AU 9718317	A1	19970811	AU 1997-18317	19970117
AU 701132	B2	19990121		
EP 883398	A1	19981216	EP 1997-903847	19970117
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1211178	A	19990317	CN 1997-191735	19970117
CN 1086937	B	20020703		
BR 9707018	A	19990720	BR 1997-7018	19970117
JP 2000503660	T2	20000328	JP 1997-526224	19970117
CZ 291530	B6	20030312	CZ 1998-2258	19970117
NO 9803019	A	19980819	NO 1998-3019	19980629
LT 4515	B	19990625	LT 1998-91	19980709
HK 1018885	A1	20021122	HK 1999-103976	19990914

PRIORITY APPLN. INFO.: US 1996-588771 A 19960119
WO 1997-US791 W 19970117

AB Photoaging of undamaged skin due to UVB irradiation exposure is inhibited by administering an agent that inhibits at least one of (1) the activity of UVB irradiation inducible MMPs in the skin, (2) one or both of the transcription factors AP-1 and NF-κB or (3) at least one of the GTP binding proteins or kinases involved in the activation and/or production of jun of fos proteins that comprise AP-1; and topically administering said inhibitor to the skin prior to such exposure. A solution of 0.1% all-trans retinoic acid (I) in 70% ethanol and 30% propylene glycol was applied to the skin of volunteers for 48 h, the skin sites were then irradiated with 2 minimal erythema dose (1 MED = 30-50 mJ/cm2). I reduced UVB-induced MMP-1 and MMP-9 mRNAs, proteins and activity by 50-80%.
IT **111753-73-2**, e5510
RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(inhibition of skin photoaging by inhibitors of matrix metalloproteinase production)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 30 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



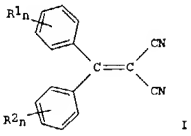
L6 ANSWER 31 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:384203 CAPLUS
DOCUMENT NUMBER: 127:23504
TITLE: Diphenyldicyanoethene-containing light-stable UV-A filters in sunscreens
INVENTOR(S): Holderbaum, Martin; Aumueller, Alexander; Sperling, Karin; Westenfelder, Horst; Wuensch, Thomas
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 10 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19540952	A1	19970507	DE 1995-19540952	19951103
CA 2234121	AA	19970515	CA 1996-2234121	19961025
WO 9717054	A1	19970515	WO 1996-EP4637	19961025
W: AU, CA, JP, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9674919	A1	19970529	AU 1996-74919	19961025
AU 706868	B2	19990624		
EP 858318	A1	19980819	EP 1996-937228	19961025
EP 858318	B1	20010606		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE, PT, IE				
JP 11514655	T2	19991214	JP 1996-517790	19961025
ES 2158358	T3	20010901	ES 1996-937228	19961025
PT 858318	T	20011030	PT 1996-937228	19961025
US 6007828	A	19991228	US 1998-68008	19980429

PRIORITY APPLN. INFO.: DE 1995-19540952 A 19951103
WO 1996-EP4637 W 19961025

OTHER SOURCE(S): MARPAT 127:23504
GI



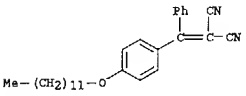
I

AB Diphenyldicyanoethenes I (R2 = C1-18 aliphatic or cycloaliph. in 2- or 4-position, C3-12 alkoxy in 4-position; R1 = H, R2; n = 1, 2) are UV-A filters which can protect skin from UV radiation in the wavelength range >320 nm. Combination of I with UV-B filters in cosmetic compns. are effective sunscreens which are resistant to photochem. decomposition I are prepared by condensation of an alkylated benzophenone with malonodinitrile in the presence of NH4OAc/HOAc (1:4) as catalyst. Thus, a water-resistant sun cream contained octyl methoxycinnamate 8.00, ethoxylated hydrogenated castor oil 5.00, propylene glycol 5.00, iso-Pr palmitate 4.00, caprylic/capric triglyceride 4.00, I (R1 = R2 = 4-OPr, n = 1) 0.5-10, glycerin 4.00, jojoba oil 3.00, 4-methylbenzylidenecamphor 2.00, TiO2 2.00, PEG-45/dodecyl glycol copolymer 1.50, dimethicone 1.50, MgSO4 0.70, Mg stearate 0.50, fragrance 0.15, and water to 100 parts.

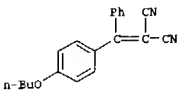
L6 ANSWER 31 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

IT **190316-21-3 190316-22-4 190316-23-5**
190316-24-6
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(diphenyldicyanoethene-containing light-stable UV-A filters in sunscreens)

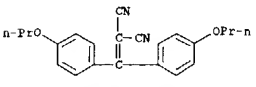
RN 190316-21-3 CAPLUS
CN Propanedinitrile, [[4-(dodecyloxy)phenyl]phenylmethylene]- (9CI) (CA INDEX NAME)



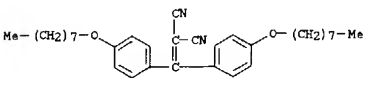
RN 190316-22-4 CAPLUS
CN Propanedinitrile, [(4-butoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)



RN 190316-23-5 CAPLUS
CN Propanedinitrile, [bis(4-propoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



RN 190316-24-6 CAPLUS
CN Propanedinitrile, [bis[4-(octyloxy)phenyl]methylene]- (9CI) (CA INDEX NAME)



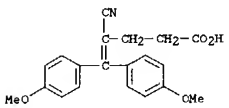
L6 ANSWER 31 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L6 ANSWER 32 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:229280 CAPLUS
DOCUMENT NUMBER: 126:272085
TITLE: Multicenter trial of the therapeutic effect of a newly developed antiplatelet agent, satigrel, on biopsy-proven chronic rejection after kidney transplantation
AUTHOR(S): Teraoka, S.; Ota, K.; Tanabe, K.; Takahashi, K.; Toma, H.; Yasumura, T.; Yoshimura, N.; Oka, T.; Takahara, S.; et al.
CORPORATE SOURCE: Tokyo Women's Medical College, Tokyo, Kyoto Prefectural University of Medicine, Kyoto, Japan
SOURCE: Transplantation Proceedings (1997), 29(1/2), 266-271
CODEN: TRPPA8; ISSN: 0041-1345
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

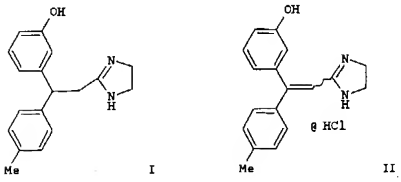
AB In conclusion, of 25 patients who developed the progressive graft dysfunction caused by biopsy-proven chronic vascular rejection, the improvement in graft function and the slowed progression of graft dysfunction were obtained during the treatment with satigrel in six and nine patients, resp., whereas graft function deteriorated again after the discontinuation of satigrel.

IT **111753-73-2**, Satigrel
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(multicenter trial of therapeutic effect of a newly developed antiplatelet agent, satigrel, on biopsy-proven chronic rejection after kidney transplantation in humans)

RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



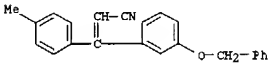
L6 ANSWER 33 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:152859 CAPLUS
DOCUMENT NUMBER: 126:238340
TITLE: Synthesis and biological evaluation of bioisosteric analogs of phentolamine
AUTHOR(S): Hog, Seoung-Soo; Lee, Heesoon; Miller, Duane D.
CORPORATE SOURCE: Coll. Pharmacy, Chungbuk Natl. Univ., 360-763, S. Korea
SOURCE: Medicinal Chemistry Research (1997), 7(1), 53-65
CODEN: MCREEB; ISSN: 1054-2523
PUBLISHER: Birkhaeuser
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The synthesis and biol. evaluation of bioisosteric analogs I and (E)- and (Z)-II, of phentolamine, is discussed. Replacement of the nitrogen with a carbon atom at the benzylic position of phentolamine shows the importance of the nitrogen atom of phentolamine for alpha-adrenergic antagonist activity; however, the ethylene analog having the Z configuration was only 15-fold less potent than phentolamine in inhibiting specific [3H]prazosin binding (alpha-1 activity) and showed considerably increased alpha-1 selectivity compared with phentolamine.

IT **188480-32-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and adrenergic antagonist activity of phentolamine analogs)

RN 188480-32-2 CAPLUS
CN 2-Propenenitrile, 3-(4-methylphenyl)-3-[3-(phenylmethoxy)phenyl]- (9CI) (CA INDEX NAME)



L6 ANSWER 33 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

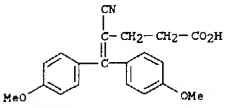
L6 ANSWER 34 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:44461 CAPLUS
DOCUMENT NUMBER: 126:65396
TITLE: Use of satigrel and aspirin as an angiogenesis inhibitor
INVENTOR(S): Kon, Kazunori; Fujiwara, Takashi
PATENT ASSIGNEE(S): Eisai Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08268886	A2	19961015	JP 1995-74744	19950331
PRIORITY APPLN. INFO.:			JP 1995-74744	19950331

AB A composition containing satigrel, aspirin, and/or pharmaceutically acceptable
salts thereof as an active ingredient is effective for the treatment of malignant tumors, keloids, inflammations, and diabetic retinopathy. A tablet containing 1 mg satigrel was formulated. Administration of satigrel Na
at 1.7 or 17 μg/kg to rabbits showed anti-angiogenic effects.

IT **111753-73-2**, Satigrel
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(satigrel and/or aspirin as angiogenesis inhibitor)

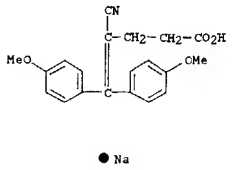
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



IT **185245-62-9**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(use of satigrel and aspirin as angiogenesis inhibitor)

RN 185245-62-9 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)-, sodium salt (9CI) (CA INDEX NAME)

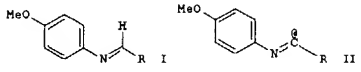
L6 ANSWER 34 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



● Na

L6 ANSWER 35 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

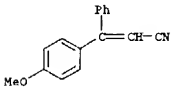
ACCESSION NUMBER: 1997:23061 CAPLUS
DOCUMENT NUMBER: 126:157256
TITLE: Isonitriles as source and fate of imidoyl radicals: a novel homolytic α-fragmentation
AUTHOR(S): Nanni, Daniele; Pareschi, Patrizia; Tundo, Antonio
CORPORATE SOURCE: Dip. Chimica organica "A. Mangini", Univ. Bologna, Bologna, I-40136, Italy
SOURCE: Tetrahedron Letters (1996), 37(52), 9337-9340
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB The compds. I R = (cyanoalkyl, alkyl, etc.) were precursors for imidoyl radicals II (same R). The reaction of imidoyl radicals II with phenylacetylene gave annulation products and a nitrile, arising from β-scission of the intermediate iminyl radical that is involved in the rearrangement of an azaspirocyclohexadienyl intermediate. In contrast, the imidoyl radical derived from N-(2,2,2-triphenylethylidene)-1-dodecanamine did not react with the alkyne and give good yields of the corresponding isonitriles through a novel example of homolytic α-fragmentation.

IT **186753-95-7**
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative) (preparation and fragmentation reaction of imidoyl radicals)

RN 186753-95-7 CAPLUS
CN 2-Propenenitrile, 3-(4-methoxyphenyl)-3-phenyl- (9CI) (CA INDEX NAME)



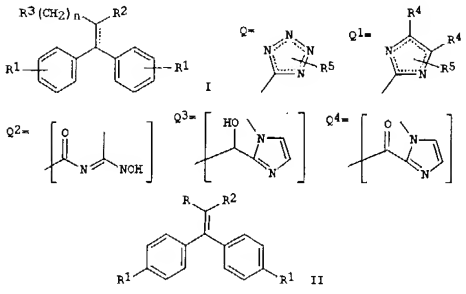
REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L6 ANSWER 36 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:18108 CAPLUS
DOCUMENT NUMBER: 126:74844
TITLE: Preparation of 1,1-diphenyl-2-heterocyclyl-1-ethylene and 3,3-diphenylethylene derivatives for activating acetylcholine, monoamines, and serotonin
INVENTOR(S): Senaga, Masahiro; Iimura, Yoichi; Sasaki, Atsushi; Kawano, Koki; Kimura, Teiji; Nakamoto, Kazutaka; Ozasa, Takashi; Furuya, Yoshiaki; Ogura, Hiroo
PATENT ASSIGNEE(S): Eisai Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 39 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08268949	A2	19961015	JP 1995-71399	19950329
PRIORITY APPLN. INFO.:			JP 1995-71399	19950329

OTHER SOURCE(S): MARPAT 126:74844
GI



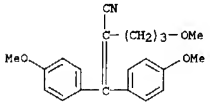
AB The title compds. [I; R1 = H, halo, OH, NH2, lower alkyl, mono- or di(lower alkyl)amino, cyano, lower halo-, cyano-, or hydroxyalkyl, lower alkyl alkoxy, etc.; R2 = lower alkoxycarbonyl, (un)substituted CONH2, lower hydroxyiminoalkyl, hydroxy(amino)imino, lower aminoalkyl, lower alkylthio, alkylsulfinyl, or alkylsulfonyl, (un)substituted heteroaryl, dimethylaminoimino, (4-ethylpiperazin-1-yl)carbonyl, Q = Q4; wherein R4, R5 = H, lower (hydroxy)alkyl; R6 = lower alkoxy, CO2H, lower alkoxycarbonyl, cyano, NH2, mono- or di(lower alkyl)amino, HO, H, halo, etc.; R3 = H, lower alkyl, alkoxy, acyl, alkylsulfonyl, or hydroxyalkoxy, (un)substituted CONH2, cyano, NH2, mono- or di(lower alkyl)amino, lower alkylthio, alkylcarbamoyloxy, or acyloxy, (un)substituted

L6 ANSWER 36 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

heteroarylalkylcarbonyl, (4-ethylpiperazin-1-yl)carbonyl; n = 0, 1-4] are prepd. These compds. are useful for prevention and treatment of dementia including dementia caused by disorders of brain blood vessels, senile dementia, Alzheimer-type dementia. Thus, Bu3SnN3 was added to Me 4-cyano-5,5-bis(4-methoxyphenyl)-4-pentenoate and stirred at 110° for 36 h to give Me 5,5-diphenyl-4-(5-tetrazolyl)pentenoate (II; R = MeO2C CH2CH2, R1 = OMe, R2 = 5-tetrazolyl). The latter compd. and II.HCl (R = BuCO, R1 = H, R2 = 4-pyridyl) increased KCl-stimulated release of acetylcholine from rat cerebral cortex slice by 152 and 352%, resp.

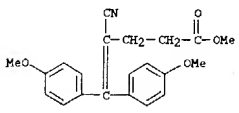
IT **184962-56-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of diphenylheterocyclylethylene and diphenylethylene derivs. for activating acetylcholine, monoamines, and serotonin for treatment of dementia)

RN 184962-56-9 CAPLUS
CN Pentanenitrile, 2-[bis(4-methoxyphenyl)methylene]-5-methoxy- (9CI) (CA INDEX NAME)



IT **184962-74-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of diphenylheterocyclylethylene and diphenylethylene derivs. for activating acetylcholine, monoamines, and serotonin for treatment of dementia)

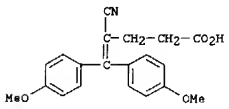
RN 184962-74-1 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 37 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:746440 CAPLUS
DOCUMENT NUMBER: 126:37141
TITLE: Polyester block copolymers containing platelet aggregation inhibitors for manufacturing antithrombotic medical goods
INVENTOR(S): Iguchi, Seiichiro; Inai, Masatoshi; Yamato, Minoru; Tono, Rika
PATENT ASSIGNEE(S): Otsuka Seiyaku Kojo Kk, Japan; Otsuka Pharma Co Ltd
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08252308	A2	19961001	JP 1996-2574	19960110
PRIORITY APPLN. INFO.:			JP 1995-7512	19950120

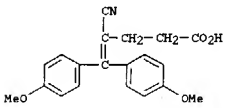
AB Polyester block copolymers such as Hytrel 4057 [comprising hard segments (polyesters) and soft segments] containing dispersed platelet aggregation inhibitors selected from cilostazol, beraprost, dipyridamol and satigrel for manufacturing antithrombotic medical goods (e.g. surgical catheters) are claimed. The materials showed slow-release of the platelet aggregation inhibitor contents.
IT **111753-73-2**, Satigrel
RL: DEV (Device component use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(polyester block copolymers containing platelet aggregation inhibitors for manufacturing antithrombotic medical goods)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 38 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:746439 CAPLUS
DOCUMENT NUMBER: 126:37140
TITLE: Polyamide block copolymers containing platelet aggregation inhibitors for manufacturing antithrombotic medical goods
INVENTOR(S): Iguchi, Seiichiro; Inai, Masatoshi; Yamato, Minoru; Tono, Rika
PATENT ASSIGNEE(S): Otsuka Seiyaku Kojo Kk, Japan; Otsuka Pharma Co Ltd
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

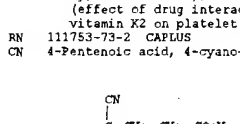
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08252307	A2	19961001	JP 1996-2573	19960110
PRIORITY APPLN. INFO.:			JP 1995-7511	19950120

AB Polyamide block copolymers such as Pebax 6333 [comprising hard segments (polyamides) and soft segments] containing dispersed platelet aggregation inhibitors selected from cilostazol, beraprost, dipyridamol and satigrel for manufacturing antithrombotic medical goods (e.g. stents) are claimed. The materials showed slow-release of the platelet aggregation inhibitor contents.
IT **111753-73-2**, Satigrel
RL: DEV (Device component use); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(polyamide block copolymers containing platelet aggregation inhibitors for manufacturing antithrombotic medical goods)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 39 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:684238 CAPLUS
DOCUMENT NUMBER: 125:316252
TITLE: Effect of drug interaction between platelet aggregation inhibitors and vitamin K2 on platelet aggregation
AUTHOR(S): Nakajima, Yoshikage; Kawashima, Hidetoshi; Takahashi, Sumiko; Nakamura, Tetsuya; Tajima, Tetsuya
CORPORATE SOURCE: Department of Applied Drug Research, Eisai Co., Ltd., Tokyo, 112, Japan
SOURCE: Iyakuhin Kenkyu (1996), 27(10), 681-687
CODEN: IYKEDH; ISSN: 0287-0894
PUBLISHER: Nippon Koteisho Kyokai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

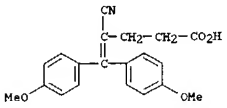
AB The effect of drug interaction between platelet aggregation inhibitors and vitamin K2 (menatetrenone, VK2) on platelet aggregation was studied in rats and guinea pigs. VK2 at 1+10-5 M did not influence collagen-induced human platelet aggregation in vitro, and an oral administration of VK2 did not show nay effect on ADP-induced platelet aggregation in rats. Further, oral administration of VK2 at a dose of 100 mg/kg did not have any effect on the inhibition of ADP-induced platelet aggregation by ticlopidine in rats. An i.m. administration of VK2 at a dose of 30 mg/kg did not show any effect on the inhibition of collagen-induced platelet aggregation by either aspirin or E-5510, a novel antiplatelet agent, in guinea pigs. In repeated administration of VK2 at a dose of 60 mg/kg/day given with the diet for 7 days, there was no difference in the percent inhibition of ADP-induced platelet aggregation by ticlopidine between VK2-treated and non-treated rats. These findings suggest that there is no drug interaction between antiplatelet and VK2, at least from the viewpoint of platelet aggregation.
IT **111753-73-2**, E-5510
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(effect of drug interaction between platelet aggregation inhibitors and vitamin K2 on platelet aggregation)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 40 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:381852 CAPLUS
DOCUMENT NUMBER: 125:104649
TITLE: Mechanisms of satigrel (E5510), a new anti-platelet drug, in inhibiting human platelet aggregation. Selectivity and potency against prostaglandin H synthases isoenzyme activities and phosphodiesterase isoform activities
AUTHOR(S): Nagakura, Naoki; Saeki, Takao; Harada, Koukichi; Yoshitake, Shinji; Kobayashi, Seiichi; Yamanaka, Takashi; Saito, Isao
CORPORATE SOURCE: Tsukuba Res. Labs., Eisai Co., Ltd., Ibaraki, 300-26, Japan
SOURCE: Biological & Pharmaceutical Bulletin (1996), 19(6), 828-833
CODEN: BPBLEO; ISSN: 0918-6158
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English

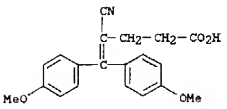
AB Satigrel (E5510,4-cyano-5,5-bis(4-methoxyphenyl)-4-pentenoic acid) is a potent inhibitor of platelet aggregation. Like cyclooxygenase/prostaglandin H synthase (PGHS) inhibitors such as aspirin, which suppress platelet aggregation by inhibiting thromboxane A2 production, satigrel inhibits collagen- and arachidonic acid-induced aggregation of human platelets. In contrast to other PGHS inhibitors, satigrel, like cyclic nucleotide phosphodiesterase (PDE) inhibitors such as cilostazol, shows inhibitory activity against thrombin-induced platelet aggregation. To investigate the mechanism of the anti-platelet activity of satigrel, we examined the selectivity and potency of satigrel against PGHS isoenzyme activities and PDE isoform activities. Two isoenzymes of PGHS are known; constitutive enzyme (PGHS1) and inducible enzyme (PGHS2). Satigrel showed inhibitory activity against PGHS1 (IC50: 0.081 μM) and PGHS2 (IC50: 5.9 μM), suggesting the selective inhibition of PGHS1. Indomethacin, which is a selective inhibitor of PGHS1, showed similar selectivity against PGHS isoenzymes (IC50: 0.12 μM and 1.4 μM, resp.). These results support that satigrel suppresses thromboxane A2 production by inhibiting PGHS1. It is known that three isoenzymes of PDE exist in human platelets: type V, which specifically hydrolyzes guanosine 3',5'-cyclic monophosphate (cGMP), Type III, which mainly hydrolyzes cAMP, and Type II, which hydrolyzes both cGMP and cAMP. We separated, these three isoenzymes from human platelets and examined the inhibitory activity of satigrel against each enzyme. Of the three isoenzymes, the inhibitory activity of satigrel was the most potent against Type III PDE (IC50: 15.7 μM). The IC50 value for Type III corresponded with that for thrombin-induced platelet aggregation. Type V and Type II were also inhibited by satigrel (IC50: 39.8 and 62.4 μM, resp.). In human platelets, satigrel increased both cAMP and cGMP levels in a dose-dependent manner (100, 300 μM). In conclusion, satigrel inhibits collagen- and arachidonic acid-induced platelet aggregation through preventing thromboxane A2 synthesis by selective inhibition of the target enzyme, PGHS1, which exists in platelets. The anti-aggregating activity of satigrel against thrombin-induced aggregation may be due to elevation of the cyclic nucleotide levels through the inhibition of PDE isoenzymes.
IT **111753-73-2**, Satigrel
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(satigrel inhibits blood platelet aggregation and alters prostaglandin H synthase and phosphodiesterase activities)
RN 111753-73-2 CAPLUS

L6 ANSWER 40 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

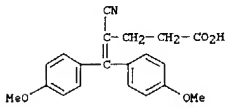


L6 ANSWER 41 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:347150 CAPLUS
DOCUMENT NUMBER: 125:48804
TITLE: Effect of E5510 on anastomotic intimal hyperplasia and platelet aggregation in dogs
AUTHOR(S): Fujioka, K.; Esato, K.; Furutani, A.; Akiyama, N.; Yoshimura, K.; Takenaka, H.; Sekido, T.; Suganuma, A.; Sagami, F.
CORPORATE SOURCE: First Dep. Surgery, Yamaguchi Univ. Sch. Med., Yamaguchi, Japan
SOURCE: Journal of Cardiovascular Pharmacology (1996), 27(6), 824-830
CODEN: JCPCDT; ISSN: 0160-2446
PUBLISHER: Lippincott-Raven
DOCUMENT TYPE: Journal
LANGUAGE: English
AB We examined the effect of an antiplatelet agent, E5510, which inhibits both platelet aggregation and release of platelet-derived growth factor (PDGF), on anastomotic intimal hyperplasia and platelet aggregation. Twenty Beagle dogs underwent infrarenal aortic reconstruction with an expanded polytetrafluoroethylene (ePTFE) graft 5 mm in diameter and 3 cm long. The dogs were divided into three groups: placebo (control group, 7 dogs), E5510 1 mg/day (1-mg group, 6 dogs), and E5510 4 mg/day (4-mg group, 7 dogs), E5510 was administered orally 2 h before operation and once daily for 3 mo after operation. Grafts were harvested 3 mo after operation. All 13 grafts in the treated groups remained patent without evidence of intimal hyperplasia, whereas only 4 of 7 grafts (57%) remained patent in the control group, including 1 graft with > 50% stenosis. Three occluded grafts showed severe intimal hyperplasia at the anastomoses. The platelet aggregation ratio (PAR) with collagen (100 μg/mL) before drug administration at 3 mo in the 4-mg group was significant lower than that in the control and 1-mg groups. PAR after drug administration at 3 mo in the 1- and 4-mg groups was significantly lower than that in the control group. Intimal thickness at the distal anastomosis was 817±190 μm in the control group, 240±80 μm in the 1-mg group, and 197±28 μm in the 4-mg group. Intimal thickness in the control group was significantly greater than that in the 1- and 4-mg groups. Smooth muscle cell (SMC) values in the intima at the distal anastomosis were 65.6±4.4% extinction (%E) in the control group, 47.6±3.4%E in the 1-mg group, and 51.3±3.5%E in the 4-mg group. SMC value in the control group was significantly greater than that in the 1- and 4-mg groups. E5510 inhibited PAR and reduced the degree of anastomotic intimal hyperplasia.
IT **111753-73-2**, E5510
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(E5510 inhibits anastomotic intimal hyperplasia and platelet aggregation in dogs after infrarenal aortic reconstruction with an expanded polytetrafluoroethylene graft)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

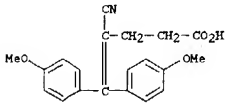
L6 ANSWER 41 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L6 ANSWER 42 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:294010 CAPLUS
DOCUMENT NUMBER: 125:58041
TITLE: Synthesis of 14C-labeled satigrel
AUTHOR(S): Tanaka, Shigeru; Yamagishi, Youji; Kusano, Kazutomi; Yoshimura, Tsutomu
CORPORATE SOURCE: Tsukuba Res. Lab., Eisai Co., Ltd., Ibaraki, 300-26, Japan
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (1996), 38(5), 435-440
CODEN: JLCRD4; ISSN: 0362-4803
PUBLISHER: Wiley
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 14C-labeled satigrel, or 4-cyano-5-(4'-methoxy [ring-U-14C]phenyl)-5-(4''-methoxyphenyl)-4-pentenoic acid was synthesized for drug metabolism and pharmacokinetic studies using 4,4'-dimethoxy[ring-U-14C]benzophenone as the starting material. The radiochem. yield was 10.0%. The specific radioactivity and radiochem. purity, as determined by radio-HPLC anal., were 10.3 MBq(277.2 μCi)/mg and 98.8%, resp.
IT **111753-73-2P**, Satigrel **178183-31-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of [14C]-satigrel)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 178183-31-8 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)-, labeled with carbon-14 (9CI) (CA INDEX NAME)

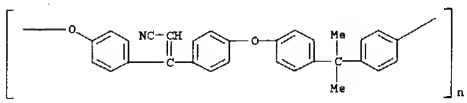


L6 ANSWER 43 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1996:255087 CAPLUS
DOCUMENT NUMBER: 125:11641
TITLE: Poly(aryl ether)s containing cyano groups
AUTHOR(S): Yeomans, Kevin A.; Hay, Allay S.
CORPORATE SOURCE: Dep. of Chemistry, McGill Univ., Montreal, QC, H3A 2K6, Can.
SOURCE: Polymeric Materials Science and Engineering (1993), 69, 240-1
CODEN: PMSEDG; ISSN: 0743-0515
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

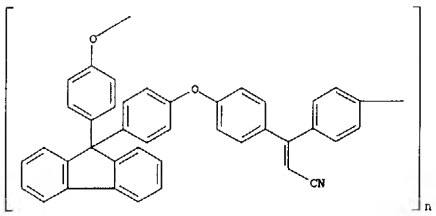
AB Poly(aryl ethers) were prepd from 3,6-difluoro-9,10-dicyanophenanthrene, 2,3-bis-4(fluorophenyl)-2-bitenedinitrile, 3,3-bis-(4-fluorophenyl)propenoic carbonitrile, and bis-(4-fluorophenyl)-methyleneppropane dinitrile and arom dialcs. Polymers were characterized.

IT **177607-57-7P 177607-59-9P 177607-61-3P**
177607-63-5P 177607-65-7P
RL: MSC (Miscellaneous); SPN (Synthetic preparation); PREP (Preparation)
(preparation and characterization of poly(aryl ether)s containing cyano groups)

RN 177607-57-7 CAPLUS
CN Poly[oxy-1,4-phenylene(cyanoethenylidene)-1,4-phenyleneoxy-1,4-phenylene(1-methylethylidene)-1,4-phenylene] (9CI) (CA INDEX NAME)

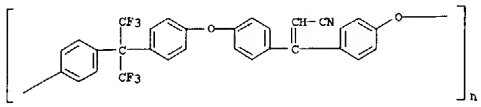


RN 177607-59-9 CAPLUS
CN Poly[oxy-1,4-phenylene-9H-fluoren-9-ylidene-1,4-phenyleneoxy-1,4-phenylene(cyanoethenylidene)-1,4-phenylene] (9CI) (CA INDEX NAME)

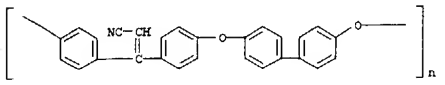


L6 ANSWER 43 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

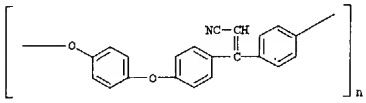
RN 177607-61-3 CAPLUS
CN Poly[oxy-1,4-phenylene(cyanoethenylidene)-1,4-phenyleneoxy-1,4-phenylene[2,2,2-trifluoro-1-(trifluoromethyl)ethylidene]-1,4-phenylene] (9CI) (CA INDEX NAME)



RN 177607-63-5 CAPLUS
CN Poly[oxy[1,1'-biphenyl]-4,4'-diyloxy-1,4-phenylene(cyanoethenylidene)-1,4-phenylene] (9CI) (CA INDEX NAME)



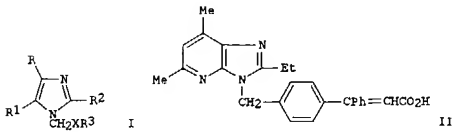
RN 177607-65-7 CAPLUS
CN Poly[oxy-1,4-phenyleneoxy-1,4-phenylene(cyanoethenylidene)-1,4-phenylene] (9CI) (CA INDEX NAME)



L6 ANSWER 44 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:946822 CAPLUS
DOCUMENT NUMBER: 123:340129
TITLE: New imidazopyridine derivatives as angiotensin II antagonists.
INVENTOR(S): Almansa, Carmen; Carceller, Elena; Gonzalez, Concepcion S.; Torres, M. Carmen; Bartroli, Javier
PATENT ASSIGNEE(S): Uriach, J., Spain; Cia, S. A.
SOURCE: Eur. Pat. Appl., 78 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 669333	A1	19950830	EP 1995-102658	19950224
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
ES 2079315	A1	19960101	ES 1994-364	19940224
ES 2079315	B1	19961016		
CA 2143412	AA	19950825	CA 1995-2143412	19950223
NO 9500684	A	19950825	NO 1995-684	19950223
JP 07267951	A2	19951017	JP 1995-61678	19950224
US 5554624	A	19960910	US 1995-393981	19950224
PRIORITY APPLN. INFO.:			ES 1994-364	19940224
OTHER SOURCE(S):		MARPAT 123:340129		

GI

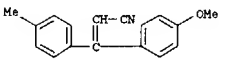


AB Imidazopyridines I [RR1 = atoms required to complete a pyridine ring; X = C6H4, pyridylene; R2 = alkyl, cycloalkyl; R3 = substituted alkyl, alkenyl] (95 compds.) were prepared for use as angiotensin II antagonists (no data). Thus, CH2(OMe)2 was treated with EtO2CCH2P(O)(OEt)2 and 4-MeC6H4COPh to give Et 3-(4-methylphenyl)-3-phenyl-2-propenoate as a cis-trans mixture, which was converted to the bromomethyl compound and treated with 5,7-dimethyl-2-ethylimidazo[4,5-b]pyridine, followed by ester hydrolysis to give imidazopyridine II.

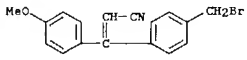
IT **170789-36-3P 170789-41-0P 170789-46-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of imidazopyridine derivs. as angiotensin II antagonists)

RN 170789-36-3 CAPLUS
CN 2-Propenenitrile, 3-(4-methoxyphenyl)-3-(4-methylphenyl)- (9CI) (CA INDEX NAME)

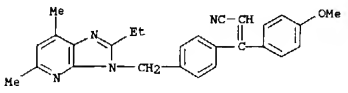
L6 ANSWER 44 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 170789-41-0 CAPLUS
CN 2-Propenenitrile, 3-[4-(bromomethyl)phenyl]-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 170789-46-5 CAPLUS
CN 2-Propenenitrile, 3-[4-[(2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridin-3-yl)methyl]phenyl]-3-(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



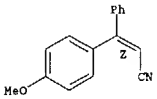
L6 ANSWER 45 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:745940 CAPLUS
DOCUMENT NUMBER: 123:338804
TITLE: Radical annulations and cyclizations with isonitriles: the fate of the intermediate imidoyl and cyclohexadienyl radicals
AUTHOR(S): Nanni, Daniele; Pareschi, Patrizia; Rizzoli, Corrado; Sgarabotto, Paolo; Tundo, Antonio
CORPORATE SOURCE: Dip. Chim. Org. "A. Mangini", Univ. Bologna, Bologna, I-40136, Italy
SOURCE: Tetrahedron (1995), 51(33), 9045-62
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The reaction of 4-methoxyphenyl isonitrile with phenylacetylene and AIBN produces a novel cyclopenta-fused quinoxaline through addition of 2-cyanoprop-2-yl radical to the alkyne; the resulting vinyl radical attacks the isonitrile to afford an imidoyl radical, which gives rise to a tandem 5-exo,6-endo cyclization. The whole process is a new example of a rare 4 + 1 radical annulation. The cyanopropyl radical can also attack the isonitrile to yield small amts. of quinolines arising from 4 + 2 and 3 + 2 annulation between the resulting imidoyl radicals and phenylacetylene. The oxidation step leading to the final aromatic products involves the starting isonitrile, which is converted to an α-unsubstituted imidoyl radical and affords 2-unsubstituted quinolines. This behavior was also found in cyclizations of biphenyl-2-yl isonitrile under various radical conditions. Finally, the title reaction gives small amts. of an α,β-unsatd. nitrile, which can arise from a spirocyclohexadienyl radical through fragmentation and subsequent β-scission of the resulting iminyl. This could be the first direct evidence of the intermediacy of iminyl radicals in the rearrangements of the spirocyclohexadienyls obtained by 3 + 2 annulation between imidoyl radicals and alkynes.

IT **170879-10-4P 170879-13-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(imidoyl and spirocyclohexadienyl radicals in annulations and cyclizations with isonitriles)

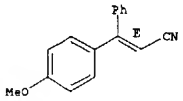
RN 170879-10-4 CAPLUS
CN 2-Propenenitrile, 3-(4-methoxyphenyl)-3-phenyl-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 170879-13-7 CAPLUS
CN 2-Propenenitrile, 3-(4-methoxyphenyl)-3-phenyl-, (2E)- (9CI) (CA INDEX NAME)

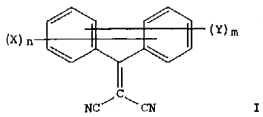
L6 ANSWER 45 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
Double bond geometry as shown.



L6 ANSWER 46 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:580750 CAPLUS
DOCUMENT NUMBER: 122:326459
TITLE: Positively charging electrophotographic photoreceptor
INVENTOR(S): Hirose, Hisahiro; Fujimoto, Shingo; Ooshiba, Tomomi; Hai, Genko
PATENT ASSIGNEE(S): Konishiroku Photo Ind, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 39 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07056366	A2	19950303	JP 1993-197499	19930809
PRIORITY APPLN. INFO.:			JP 1993-197499	19930809

OTHER SOURCE(S): MARPAT 122:326459
GI

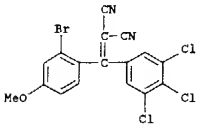


I

AB The title electrophotog. photoreceptor utilizes as charge-transporting material,[I; Y = CN, halo; m ≥ 3 (when m = 3, Ys are identical; when m ≥ 4, Ys may not be identical); X = R1, COR1, COOR1, SOR1, SO2R1, CONHR1, CR2:CR2R1, SO2NHR1, OR1, Ph; n ≥ 0; R1 = alkyl, phenyl; R2 = H, R1].

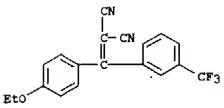
IT **163450-37-1 163450-54-2**
RL: DEV (Device component use); USES (Uses)
(charge-transporting material; for electrophotog. photoreceptor)

RN 163450-37-1 CAPLUS
CN Propanedinitrile, [(2-bromo-4-methoxyphenyl)(3,4,5-trichlorophenyl)methylene]- (9CI) (CA INDEX NAME)

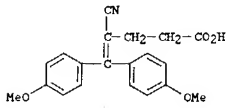


RN 163450-54-2 CAPLUS
CN Propanedinitrile, [(4-ethoxyphenyl)[3-(trifluoromethyl)phenyl]methylene]- (9CI) (CA INDEX NAME)

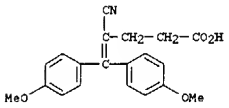
L6 ANSWER 46 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



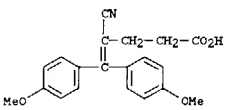
L6 ANSWER 47 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:516394 CAPLUS
DOCUMENT NUMBER: 122:255859
TITLE: Mutagenicity studies of E5510 (1); reversion test in bacteria
AUTHOR(S): Mochida, Hisatoshi
CORPORATE SOURCE: Department of Drug Safety Research, Eisai Co., Ltd., Japan
SOURCE: Yakuri to Chiryo (1973-2000) (1994), 22(12), 4893-7
CODEN: YACHDS; ISSN: 0386-3603
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB The mutagenicity of E5510 was tested by using Salmonella typhimurium strains and Escherichia coli. The results indicated that E5510 is nonmutagenic under present exptl. conditions.
IT **111753-73-2**, E5510
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(mutagenicity studies of E5510 (1); reversion test in bacteria)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



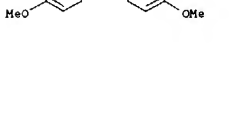
L6 ANSWER 48 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:475425 CAPLUS
DOCUMENT NUMBER: 122:255860
TITLE: Mutagenicity studies of E5510 (2) --chromosome aberration study in mammalian cultured cells--
AUTHOR(S): Sawada, Shigeki; Tanabe, Yoshio; Kondoh, Senji; Igarashi, Toshiji; Yamatsu, Kiyomi
CORPORATE SOURCE: Department of Drug Safety Research, Eisai Co., Ltd., Hashima, 501-61, Japan
SOURCE: Yakuri to Chiryo (1973-2000) (1994), 22(12), 4899-60
CODEN: YACHDS; ISSN: 0386-3603
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB Chromosome aberration study of E5510 was carried out using cultured Chinese hamster lung cells (CHL/IU cells). The cells were treated with E5510 in either direct method or S9 Mix method. E5510 at doses of 0.05-0.15 mg/mL significantly increased the incidence of aberrant cells in direct method. In S9 Mix method, E 5510 at a dose of 0.4 mg/mL significantly increased the incidence of aberrant cells and polyploid cells. Pos. controls, MNNG and DMBA, significantly increased the incidence of aberrant cells in this assay system. Therefore, E5510 was clastogenic to CHL/IU cells under the conditions of this experiment
IT **111753-73-2**, E5510
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(mutagenicity studies of E5510 (2) --chromosome aberration study in mammalian cultured cells--)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 49 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:475424 CAPLUS
DOCUMENT NUMBER: 122:255858
TITLE: Fetal ductus arteriosus constriction by E5510 in rats
AUTHOR(S): Furuhashi, Tadakazu; Kato, Masashi; Nakagawa, Ken-Ichi; Shionoya, Hiroshi; Sagami, Fumio; Noguchi, Masayoshi; Yamatsu, Kiyomi
CORPORATE SOURCE: Hashima Laboratory, Nihon Bioresearch Inc., Hashima, 501-62, Japan
SOURCE: Yakuri to Chiryo (1973-2000) (1994), 22(12), 4887-91
CODEN: YACHDS; ISSN: 0386-3603
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB Single oral administration of E5510 at doses of 0.16, 1.6 and 16 mg/kg was performed in rats during the final stage of pregnancy, and its effect on fetal ductus arteriosus constriction was evaluated at 4 h after administration. Indomethacin was used as a reference drug at a dose of 1 mg/kg. E5510 at 0.16 mg/kg had no effects on the ductus arteriosus constriction, whereas E5510 at 1.6 mg/kg or higher caused dose-dependent ductus arteriosus constriction. Indomethacin at 1 mg/kg caused marked constriction of the ductus arteriosus. Comparing the effects of E5510 at 0.16 mg/kg, the estimated clin. dosage, with those of indomethacin at 1 mg/kg, indomethacin caused marked ductus arteriosus constriction, whereas E5510 had no effects on ductus arteriosus constriction. Based on the above results, the effects of E5510 at the estimated clin. dosage on fetal ductus arteriosus constriction can be evaluated to be "nil" under the conditions of the present study, and it can be concluded that the effect of E5510 on fetal ductus arteriosus is slight.
IT **111753-73-2**, E5510
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(fetal ductus arteriosus constriction by E5510 in rats)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 50 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:475423 CAPLUS
DOCUMENT NUMBER: 122:255857
TITLE: Teratological study in rats treated orally with E5510
AUTHOR(S): Gotoh, Masataka; Ohsumi, Isamu; Nishimura, Osamu; Kawaguchi, Takashi; Okada, Fumihiro; Matsubara, Yoshio; Igarashi, Toshiji; Yamatsu, Kiyomi
CORPORATE SOURCE: Department of Drug Safety Research, Eisai Co., Ltd., Hashima, 501-61, Japan
SOURCE: Yakuri to Chiryo (1973-2000) (1994), 22(12), 4861-77
CODEN: YACHDS; ISSN: 0386-3603
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
AB A teratol. study of E 5510, a newly developed antiplatelet agent, was performed using Slc : SD rats. E 5510 at dose levels of 1, 3 and 10 mg/kg/day was orally administered to pregnant rats once a day from day 7 to day 17 of gestation, and the effects on F0 dams, F1 fetuses and F1 offspring were evaluated. In F0 dams, no effects were noted on general signs, body weight, food consumption, delivery, nursing or necropsy findings.
In F1 fetuses of the 10 mg/kg dose group, the number of ossified sacral and caudal vertebral bodies was slightly decreased. However, no effects were found on the incidences of resorptions or dead fetuses, external, internal and skeletal anomalies, sex ratio or fetal body weight In F1 offspring, no effects were found on body weight, phys. or functional development, behavioral function or reproductive function. Based on these results, the no-effect dose level of E 5510 is 10 mg/kg/day for F0 dams and their offspring and is 3 mg/kg/day for their fetuses.
IT **111753-73-2**, E5510
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(teratol. study in rats treated orally with E5510)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

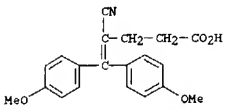


L6 ANSWER 51 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:475422 CAPLUS
DOCUMENT NUMBER: 122:255856
TITLE: E5510 subacute toxicity study in beagle dogs on repeated oral administration for 13 weeks followed by a 5-week recovery period
AUTHOR(S): Hayakawa, Kazuhiro; Noguchi, Masayoshi; Tanaka, Hisashi; Tanaka, Shigeru; Tagaya, Osamu; Tanabe, Yoshio; Nakanowatari, Jun-Ichi; Igarashi, Toshiji; Yamatsu, Kiyomi
CORPORATE SOURCE: Department of Drug Safety Research, Eisai Co., Ltd., Hashima, 501-61, Japan
SOURCE: Yakuri to Chiryo (1973-2000) (1994), 22(12), 4843-60
CODEN: YACHDS; ISSN: 0386-3603
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB E5510 is a new anti-platelet drug which inhibits both activities of cyclo-oxygenase and phosphodiesterase. The purpose of this study was to evaluate the subacute toxicity of E5510 when administered orally to beagle dogs for 13 wk. The dose levels were set at 0, 0.3, 1, 3 and 6 mg/kg/day. Three animals per sex per group were assigned to a 0.3, 1, and 3 mg/kg group, and 4 and 5 animals per sex were for control and 6 mg/kg group resp. One animal per sex from the control and two animals per sex from the 6 mg/kg group were maintained undosed for 5 wk after cessation of the dosing period to evaluate the recoverability. During the course of the study, daily observations, weekly body wts., food and water consumption, pharmacokinetics, electrocardiog., ophthalmol. examns., laboratory investigations, hepatic drug metabolizing enzyme activity and post mortem examination were utilized to detect evidence of toxicity. No treatment-related changes were found in any animals receiving 0.3 and 1 mg/kg. There were no dead animals throughout the experiment period. However one of the six animals receiving 3 mg/kg was sacrificed in extremis on day 17 of treatment because of emaciation. Examns. including microscopical and bacteriol. studies revealed that the animal died of systemic infection and lymphadenitis which presumably developed secondary to the massive bleeding from the gastrointestinal tract. All toxic findings in this repeated dose study were related to gastrointestinal ulcer formation and bleeding from the gastrointestinal tract, i.e. the ulcers were detected in three animals (including the one sacrificed in extremis) by gross and/or microscopical examination and intestinal bleeding was indicated in 10 of the 16 animals of the 3 and 6 mg/kg groups by occult blood pos. stools examined during the period of treatment, although all 20 animals in control, 0.3 and 1 mg/kg groups were neg. No gastrointestinal bleeding was found in any of the 4 animals treated with 6 mg/kg of E5510 when examined at the end of recovery period. In some animals treated with 3 or 6 mg/kg there were further changes in blood chemical parameters which were statistically but not toxicol. significant. They were decreased alkaline phosphatase (ALP) and total protein, and increased urea nitrogen. These changes were considered secondary to the gastrointestinal bleeding. Apart from the above-mentioned findings, there were no particular toxic findings in any observations and examns. The no-effect dose level was 1 mg/kg, and the toxic dose level was 3 mg/kg where gastrointestinal ulcers bleedings were found among animals.

IT **111753-73-2**, E 5510
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(E5510 subacute toxicity study in beagle dogs on repeated oral

L6 ANSWER 51 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
administration for 13 wk followed by a 5-wk recovery period)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

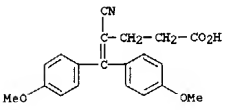


L6 ANSWER 52 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:475421 CAPLUS
DOCUMENT NUMBER: 122:255855
TITLE: E5510 toxicity study in rats on repeated oral administration for 13 weeks
AUTHOR(S): Sumigama, Shuji; Shirakabe, Atsushi; Taki, Toyohiko; Nakanowatari, Jun-Ichi; Tanabe, Yoshio; Tagaya, Osamu; Igarashi, Toshiji; Yamatsu, Kiyomi
CORPORATE SOURCE: Department of Drug Safety Research, Eisai Co., Ltd., Hashima, 501-61, Japan
SOURCE: Yakuri to Chiryo (1973-2000) (1994), 22(12), 4819-42
CODEN: YACHDS; ISSN: 0386-3603
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB E5510 is a newly developed antiplatelet agent. E5510 at dosage of 1, 3, 10 and 30 mg/kg/day was administered to male and female Sprague-Dawley rats by gavage once a day for 13 wk. Following the end of the 13-wk administration period, 10 and 30 mg/kg/day groups were kept without treatment for an addnl. 5 wk. No E5510 treatment-related mortalities were noted during the exptl. period. There were no overt toxic clin. signs in any dose levels excepting salivation after administration of higher doses (10 and 30 mg/kg/day). There were no clin. signs at any dose levels during the recovery period. Suppression of body weight gain was observed in the males and females of 30 mg/kg/day group during the treatment period. These changes recovered by the cessation of dosing. Increased incidence occult blood pos. feces were observed in some males and females in both 10 and 30 mg/kg/day groups during the first week of treatment. This change suggested gastrointestinal bleeding. There were no remarkable ophthalmol. findings in any dose levels. There were no remarkable hematol. findings in any dose levels. Decreased plasma levels of total cholesterol, HDL-cholesterol and plasma level of γ-globulin in the males of 10 mg/kg/day group. Decreased plasma level of total cholesterol, HDL-cholesterol and phospholipids in the both sexes, decreased plasma levels of urea nitrogen and γ-globulin and increased plasma levels of triglycerides and non esterified fatty acid in the males, and increased plasma level of α1-globulin and decreased plasma levels of albumin, A/G ratio and calcium in the females of 30 mg/kg/day group. These changes disappeared by the end of the recovery period. There were no remarkable urine findings in any dose levels. There were no remarkable macroscopic changes and organ weight in any dose levels. Histopathol. finding in post mortem examination was hypertrophy of adrenal cortex in the males of 10 and 30 mg/kg/day groups. This change was not detected at the end of the recovery period. Based on these results, the non-toxic dosage level was concluded to be 3 mg/kg/day.

IT **111753-73-2**, E5510
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(E5510 toxicity study in rats on repeated oral administration for 13 wk)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

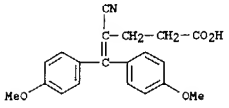
L6 ANSWER 52 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L6 ANSWER 53 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:475420 CAPLUS
DOCUMENT NUMBER: 122:255854
TITLE: Acute toxicity study of E5510 by oral administration in beagle dogs
AUTHOR(S): Noguchi, Masayoshi; Nakanowatari, Jun-Ichi; Tanabe, Yoshio; Tagaya, Osamu; Igarashi, Toshiji; Yamatsu, Kiyomi
CORPORATE SOURCE: Department of Drug Safety Research, Eisai Co., Ltd., Hashima, 501-61, Japan
SOURCE: Yakuri to Chiryo (1973-2000) (1994), 22(12), 4811-17
CODEN: YACHDS; ISSN: 0386-3603
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB E5510 was evaluated for its general toxicity potential following oral administration to male and female dogs at dosage levels of 100, 300 and 1000 mg/kg. No animals died even at the high dose. All toxic findings in this single dose study were related to gastrointestinal ulcer formation and bleeding from the gastrointestinal tract, i. e. the ulcers were detected in three animals by macro and/or microscopical examination and intestinal bleeding was indicated by reddish and/or blackish stool and occult blood pos. stools in all animals. Decreased food consumption and body weight, decreased red blood cell count, Hb and hematocrit and increased white blood cell count and erythrocyte sedimentation rate decreased and increased platelet count in hematol., decreased total protein and albumin in blood chemical were observed at 300 mg/kg and above. Other findings were increased alkaline phosphatase (ALP), triglyceride, urea nitrogen and inorg. phosphorus, and decreased glutamic-pyruvic transaminase (GPT), glutamic-oxaloacetic transaminase (GOT) and choline-esterase in blood chemical Urinalysis revealed urine glucose false pos. These changes were also considered to be related to the intestinal bleeding, because they were found together with the bleeding and there were no histopathol. findings except gastrointestinal ulcers. Food consumption and blood chemical parameters recovered on day 14, but decreased body weight, hematol. parameters (RBC, HT, HB) and gastrointestinal ulcers remained at the end of the observation.

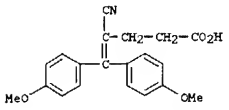
IT **111753-73-2**, E5510
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(acute toxicity study of E5510 by oral administration in beagle dogs)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 54 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:475419 CAPLUS
DOCUMENT NUMBER: 122:255853
TITLE: Acute toxicity study of E5510 by oral, intraperitoneal and subcutaneous administration in mice and rats
AUTHOR(S): Sumigama, Shuji; Shirakabe, Atsushi; Nakanowatari, Jun-ichi; Tanabe, Yoshio; Tagaya, Osamu; Miyagawa, Hidekazu; Taki, Toyohiko; Igarashi, Toshiji; Yamatsu, Kiyomi
CORPORATE SOURCE: Department of Drug Safety Research, Eisai Co., Ltd., Hashima, 501-61, Japan
SOURCE: Yakuri to Chiryo (1973-2000) (1994), 22(12), 4801-9
CODEN: YACHDS; ISSN: 0386-3603
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB E5510 is a newly developed antiplatelet agent. Acute toxicity studies were carried out using ICR mice and SD rats. Irresp. of dosing route, the mice showed hypoactivity, prone positioning and clonic convulsion after administration. The mice received orally and s.c. also showed blanched auricles. Macroscopically, gastrointestinal lesions were observed in dead animals and sacrificed animals at the end of observation period (14 days after dosing) in all routes. Irresp. of dosing route, the rats showed hypoactivity, prone positioning, lacrimation and blanched auricles after administration. The rats received orally and i.p. also showed loss of righting reflex, mydriasis and clonic convulsion. Macroscopically, gastrointestinal lesions were observed in dead animals and sacrificed animals at the end of observation period (14 days after dosing) in all routes. The acute toxicity of E5510 by i.p. and s.c. injection was qual. comparable with that by oral administration, though the onset of toxicity was rapid after i.p. administration but rather slow after s.c. administration. The development of gastrointestinal lesions is considered to be related to cyclooxygenase inhibiting action of E5510.

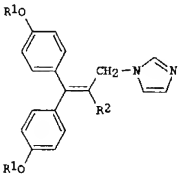
IT **111753-73-2**, E5510
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(acute toxicity study of E5510 by oral, i.p. and s.c. administration in mice and rats)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 55 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1995:308725 CAPLUS
DOCUMENT NUMBER: 122:81365
TITLE: Preparation of 1-(3,3-diphenyl-2-propenyl)imidazole derivatives as blood platelet aggregation inhibitors
INVENTOR(S): Ito, Yasuo; Kato, Hideo; Yasuda, Shingo; Ogawa, Nobuo; Suzuki, Tomio; Sakurai, Shunichiro
PATENT ASSIGNEE(S): Hokuriku Pharmaceutical, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06228106	A2	19940816	JP 1993-40673	19930205
PRIORITY APPLN. INFO.:			JP 1993-40673	19930205

OTHER SOURCE(S): MARPAT 122:81365
GI

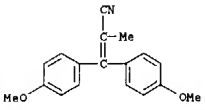


I

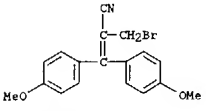
AB The title compds. (I; R1 = lower alkyl; R2 = cyano, halo), which inhibit both thromboxane A2 synthesis and cyclooxygenase and also useful as antithrombotics (no data), are prepared Thus, a mixture of 2.85 g 2-bromomethyl-3,3-bis(4-methoxyphenyl)acrylonitrile (preparation given), 1.09 g imidazole, and 8 mL toluene was stirred at 120° for 1 h to give 1.64 g title compound I (R1 = Me, R2 = cyano).

IT **161406-44-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(bromination in preparation of [bis(hydroxyphenyl)propenyl]imidazole derivs. as blood platelet aggregation inhibitors and antithrombotics)
RN 161406-44-6 CAPLUS
CN 2-Propenenitrile, 3,3-bis(4-methoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)

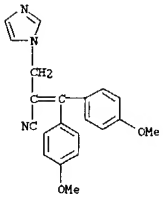
L6 ANSWER 55 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT **160413-74-1P**, 2-Bromomethyl-3,3-bis(4-methoxyphenyl)acrylonitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate for preparation of [bis(hydroxyphenyl)propenyl]imidazole derivs. as blood platelet aggregation inhibitors and antithrombotics)
RN 160413-74-1 CAPLUS
CN 2-Propenenitrile, 2-(bromomethyl)-3,3-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



IT **160413-72-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of [bis(hydroxyphenyl)propenyl]imidazole derivs. as blood platelet aggregation inhibitors and antithrombotics)
RN 160413-72-9 CAPLUS
CN 1H-Imidazole-1-propanenitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



L6 ANSWER 56 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

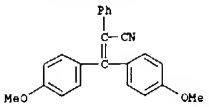
ACCESSION NUMBER: 1995:237206 CAPLUS
DOCUMENT NUMBER: 122:23229
TITLE: Study of the effects of basic di- and tri-phenyl derivatives on malignant cell proliferation: an example of the application of Correspondence Factor Analysis to structure-activity relationships (SAR)
AUTHOR(S): Gilbert, Jacques; Dore, Jean-Christophe; Bignon, Eric; Pons, Michel; Ojasoo, Tiiu
CORPORATE SOURCE: CNRS, CERCOA, Thiais, 94320, Fr.
SOURCE: Quantitative Structure-Activity Relationships (1994), 13(3), 262-74
CODEN: QSARDI; ISSN: 0931-8771
PUBLISHER: VCH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The descriptive multivariate method known as Correspondence Factor Anal. (CFA) was used to establish correlations between the structures of three chemical classes of compds. (triphenylacrylonitriles (TPEs), diphenylethylenes (DPEs), and diphenylalkyls) substituted in the para position by either hydroxy or basic groups and their responses in a battery of three biochem. tests, namely the induction of the proliferation of the MCF7 human breast cancer cell-line, the estrogen-irreversible inhibition of MCF7 cell proliferation (herein denoted cytotoxicity), and binding to the estrogen receptor (ER). The power of CFA was illustrated by performing several analyses: (a) Construction of factorial maps that described only the specificity of the response of the TPE population in the tests or both the specificity and amplitude of the response; (b) Use of the factorial maps as math. models for the introduction of new variables. These variables were either further biochem. tests (cytotoxicity under different conditions, inhibition of the activation of protein kinase C) on which the TPE population had been screened or further compds. (DPEs and diphenylalkyls). Relationships among the different tests were thus assessed as well as affiliations of the new compds. with TPEs. The analyses revealed the importance of the presence and configuration of hydroxy groups in ER binding and cell proliferation, but also the ability of non-hydroxylated compds. to induce cell growth independently of their relative affinity for ER. Cytotoxicity could be related to the presence of basic groups but also to resonance of conjugated bis-para-hydroxy di-Ph derivs. Overall, the analyses stressed the complexity of the relationships between growth-promoting and growth-inhibitor potential of the test-compound populations and suggested the involvement of multiple mechanisms of action.

IT **66422-13-7 104575-13-5 104575-22-6 118976-12-8 118976-13-9 118976-15-1 137743-23-8 137743-26-1**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(application of Correspondence Factor Anal. to structure-activity relationship of basic di- and tri-Ph derivs. on malignant cell proliferation)

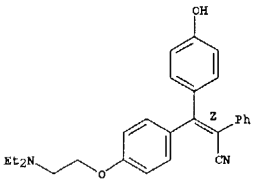
RN 66422-13-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 56 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



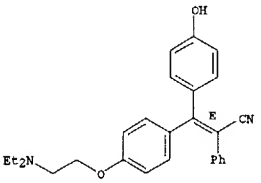
RN 104575-13-5 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 104575-22-6 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

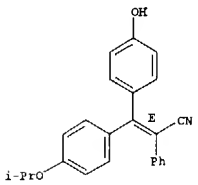
Double bond geometry as shown.



RN 118976-12-8 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)[4-(1-methylethoxy)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

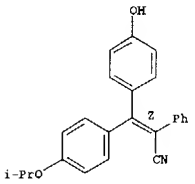
Double bond geometry as shown.

L6 ANSWER 56 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

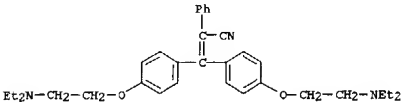


RN 118976-13-9 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)[4-(1-methylethoxy)phenyl]methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

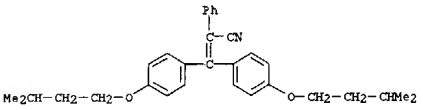


RN 118976-15-1 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-[2-(diethylamino)ethoxy]phenyl]methylene]- (9CI) (CA INDEX NAME)

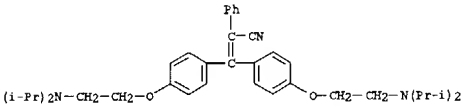


RN 137743-23-8 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-(3-methylbutoxy)phenyl]methylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 56 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



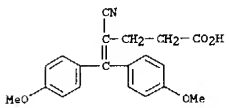
RN 137743-26-1 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-[2-[bis(1-methylethyl)amino]ethoxy]phenyl]methylene]- (9CI) (CA INDEX NAME)



L6 ANSWER 57 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:595477 CAPLUS
DOCUMENT NUMBER: 121:195477
TITLE: E5510 antagonizes thrombin receptor signals by inhibiting NF-κB activation
AUTHOR(S): Nakajima, Toshihiro; Kitajima, Isao; Shin, Hiroshi; Matsumoto, Wataru; Soejima, Yasuko; Maruyama, Ikuro
CORPORATE SOURCE: Fac. Med., Univ. Kagoshima, Kagoshima, 890, Japan
SOURCE: Biochemical and Biophysical Research Communications (1994), 203(2), 1181-7
CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB We have recently demonstrated that NF-κB is involved in a thrombin-signaling and that the antisense oligodeoxynucleotides (ODNs) of NF-κB has a marked inhibitory effect on thrombin-induced cellular responses. In this study, we demonstrate that E5510 (4-cyano-5,5-bis(methoxyphenyl)-4-pentenoic acid), a compound with antiplatelet activity preferentially inhibits the thrombin-inducible NK-κB activation and then antagonizes the following thrombin-induced cellular responses, proliferation and cytokines production in vascular smooth muscle cell and the adherence of differentiated HL-60 cells. These data suggest that E5510 has an antiatherosclerotic or antirestenotic effect.

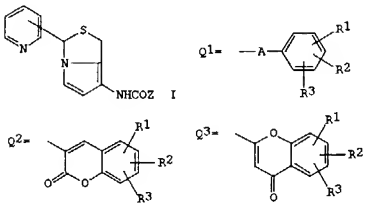
IT **111753-73-2**, E5510
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(E5510 antagonizes thrombin receptor signals by inhibiting NF-κB activation)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 58 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1994:217660 CAPLUS
DOCUMENT NUMBER: 120:217660
TITLE: Preparation of pyrrolothiazoles as pharmaceuticals
INVENTOR(S): Nagaoka, Hitoshi; Shishikura, Junichi; Tomioka, Kenichi; Mase, Toshasu
PATENT ASSIGNEE(S): Yamanouchi Pharma Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 28 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05230069	A2	19930907	JP 1992-70152	19920220
PRIORITY APPLN. INFO.:			JP 1992-70152	19920220

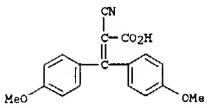
OTHER SOURCE(S): MARPAT 120:217660
GI



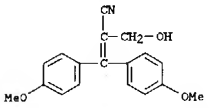
AB Pyrrolothiazoles I [Z = Q1-3; R1-3 = H, halo, lower (halo)alkyl, alkoxy, alkylthio, alkylsulfinyl, or alkylsulfonyl, OH, cyano, NO2; A = (substituted) alkylene, alkenylene, or alkynylene; if A = unsubstituted alkylene, then R1 = R2 = R3 ≠ H], their salts, stereoisomers, and solvates are prepared as platelet-activating factor antagonists and thromboxane A2 inhibitors (no data). 2-Cyano-5-(4-methoxyphenyl)-2,4-decadienoic acid (372 mg) was chlorinated with (COCl)2 in DMF-CH2Cl2 at room temperature for 1 h to give acid chloride. Sep., 400 mg I (Z = OCMe3, 3-pyridyl) was treated with CF3CO2H at room temperature for 1 h and treated with the acid chloride and NEt3 at room temperature for 12 h to give 191 mg I [Z = Q1, R1 = 4-OMe, R2 - R3 = H, A = C(CN):CHCH:C(CH2)4Me, 3-pyridyl].

IT **20168-04-1**
RL: RCT (Reactant); RACT (Reactant or reagent)
(chlorination of)
RN 20168-04-1 CAPLUS
CN 2-Propenoic acid, 2-cyano-3,3-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

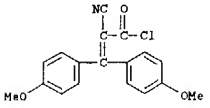
L6 ANSWER 58 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT **153530-10-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and oxidation of)
RN 153530-10-0 CAPLUS
CN 2-Propenenitrile, 2-(hydroxymethyl)-3,3-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

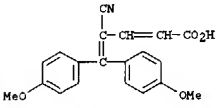


IT **153530-09-7P**, 3,3-Bis(4-methoxyphenyl)-2-cyanopropenoyl chloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
RN 153530-09-7 CAPLUS
CN 2-Propenoyl chloride, 2-cyano-3,3-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

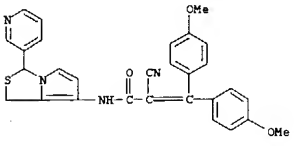


IT **153530-00-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for pyrrolothiazole pharmaceuticals)
RN 153530-00-8 CAPLUS
CN 2,4-Pentadienoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 58 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

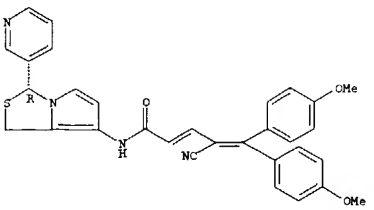


IT **153529-72-7P 153529-80-7P 153529-85-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as pharmaceutical)
RN 153529-72-7 CAPLUS
CN 2-Propenamide, 2-cyano-3,3-bis(4-methoxyphenyl)-N-[3-(3-pyridinyl)-1H,3H-pyrrolo[1,2-c]thiazol-7-yl]- (9CI) (CA INDEX NAME)



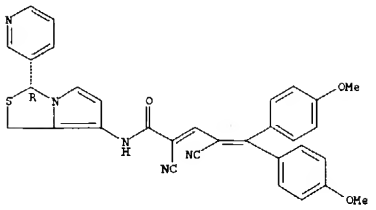
RN 153529-80-7 CAPLUS
CN 2,4-Pentadienamide, 4-cyano-5,5-bis(4-methoxyphenyl)-N-[3-(3-pyridinyl)-1H,3H-pyrrolo[1,2-c]thiazol-7-yl]-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

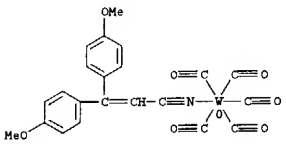


RN 153529-85-2 CAPLUS
CN 2,4-Pentadienamide, 2,4-dicyano-5,5-bis(4-methoxyphenyl)-N-[3-(3-pyridinyl)-1H,3H-pyrrolo[1,2-c]thiazol-7-yl]-, (R)- (9CI) (CA INDEX NAME)

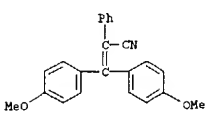
L6 ANSWER 58 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
Absolute stereochemistry.
Double bond geometry unknown.



L6 ANSWER 59 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:626125 CAPLUS
DOCUMENT NUMBER: 119:226125
TITLE: α-Addition of amines, imines, and hydrazines to allenylidene complexes - preparation of carbene, azetidinylidene, and nitrile complexes
AUTHOR(S): Fischer, Helmut; Roth, Gerhard; Reindl, David; Troll, Carsten
CORPORATE SOURCE: Fakultaet fuer Chemie, Universitaet Konstanz, Postfach 5560, Konstanz, D-78434/1, Germany
SOURCE: Journal of Organometallic Chemistry (1993), 454(1-2), 133-49
CODEN: JORCAI; ISSN: 0022-328X
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 119:226125
AB Diarylallenylidene(pentacarbonyl)chromium and -tungsten complexes, (CO)5M:C:C:CR2 (M = W (1), Cr (2)), react with amines, imines and hydrazines by addition of the nitrogen nucleophile to the Cα allenylidene atom. With NEt3 the adduct formation is reversible. With secondary and primary amines, imines and hydrazines, the initially formed N-ylide complexes react readily further to give carbene, azetidinylidene and nitrile complexes, resp. For example the reaction of (a) 1 and 2 with HNEt2 or H2NPh gives alkenyl(amino)carbene complexes, (CO)5M:C[C(H):CR2]NR'2 (3-5); (b) of 1 and 2 with HN:CR'2 gives alkenyl(alkylideneamino)carbene complexes, (CO)5M:C[C(H):CR2][N:CR'2] (6, 7); (c) of 1 with (Me2CH)N:C(Ph)H the azetidinylidene complex 9; (d) of 1 with 1,2-disubstituted hydrazines such as H(Me)NN(R)H (R = Me, Ph) alkenyl(hydrazino)carbene complexes, (CO)5W:C[C(H):CR2][N(Me)N(R)H] (11) and (e) of 1 with H2NNR1R2 (R1 = R2 = H, Me; R1 = H, R2 = Ph) alkenyl(amino)carbene complexes (13) and/or acrylonitrile complexes, (CO)5W[NCC(H):CR2] (12). The structures of representative examples of 6, 11 and 12 were established by x-ray analyses.
IT **150833-75-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 150833-75-3 CAPLUS
CN Tungsten, [3,3-bis(4-methoxyphenyl)-2-propenenitrile-N]pentacarbonyl-, (OC-6-22)- (9CI) (CA INDEX NAME)

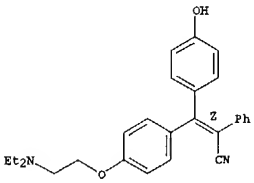


L6 ANSWER 60 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:247109 CAPLUS
DOCUMENT NUMBER: 118:247109
TITLE: Relative involvement of protein kinase C and of the estrogen receptor in the cytotoxic action of a population of triphenylethylenes on MCF7 cells as revealed by correspondence factorial (CF) analysis
AUTHOR(S): Ojasoo, Tiiu; Bignon, Eric; Crastes de Paulet, Andre; Dore, Jean Christophe; Gilbert, Jacques; Miquel, Jean Francois; Pons, Michel; Raynaud, Jean Pierre
CORPORATE SOURCE: Roussel-Uclaf, Paris, 75007, Fr.
SOURCE: Journal of Steroid Biochemistry and Molecular Biology (1993), 44(3), 239-50
CODEN: JSBBEZ; ISSN: 0960-0760
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A multivariate statistical method, correspondence factorial (CF) anal., was used to examine the correlations of protein binding and cell proliferation effects in a series of 36 diphenylethylenes and triphenylethylenes (DPEs and TPEs). The anal. was applied to a study which measured their competition for estradiol binding to cytosol estrogen receptor (ER), their influence on protein kinase C (PKC) activity under different conditions of enzyme activation, and their ability to promote the growth of the MCF7 breast cancer cell line and to inhibit growth at high concns. (cytotoxicity). The CF anal. revealed several levels of correlation. It distinguished the mols. within the population that stimulated rather than inhibited the PKC activity. It made apparent a strong correlation between the cytotoxicity and inhibition of Ca2+ and phosphatidylserine-dependent PKC activity, which was most marked when the enzyme had been activated by diacylglycerol, indicating that PKC inhibition under physiol. conditions might contribute to the overall cytotoxicity of these compds. A lower level of correlation was established between the competition for ER binding and cytotoxicity. The MCF7 cells might be most sensitive to cytotoxic effects of TPEs (via PKC and other targets) when the agents simultaneously decrease the estrogen-stimulated proliferation via an ER-mediated antiestrogenic effect.
IT **66422-13-7 104575-13-5 104575-22-6 118976-12-8 118976-13-9 118976-15-1 137743-23-8 137743-26-1**
RL: PRP (Properties)
(antitumor effects of, in mammary cancer, estrogen receptors and protein kinase C role in)
RN 66422-13-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



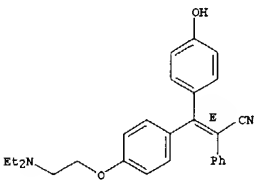
RN 104575-13-5 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

L6 ANSWER 60 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
Double bond geometry as shown.



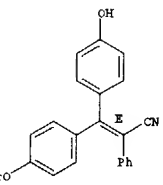
RN 104575-22-6 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 118976-12-8 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)[4-(1-methylethoxy)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

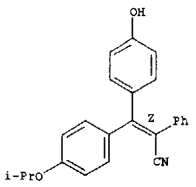
Double bond geometry as shown.



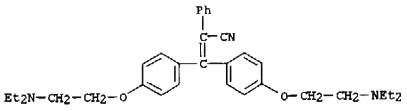
RN 118976-13-9 CAPLUS

L6 ANSWER 60 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)[4-(1-methylethoxy)phenyl]methylene]-, (Z)- (9CI) (CA INDEX NAME)

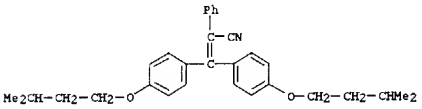
Double bond geometry as shown.



RN 118976-15-1 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-[2-(diethylamino)ethoxy]phenyl]methylene]- (9CI) (CA INDEX NAME)

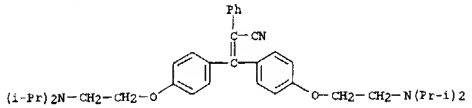


RN 137743-23-8 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-(3-methylbutoxy)phenyl]methylene]- (9CI) (CA INDEX NAME)

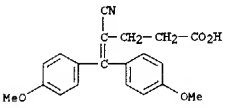


RN 137743-26-1 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-[2-[bis(1-methylethyl)amino]ethoxy]phenyl]methylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 60 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



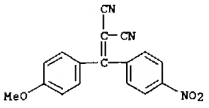
L6 ANSWER 61 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:94102 CAPLUS
DOCUMENT NUMBER: 118:94102
TITLE: Inhibitory effects of a novel antiplatelet agent, E5510, on collagen-induced platelet-derived growth factor release and aggregation of human platelets in vitro
AUTHOR(S): Nomoto, Kenichi; Saeki, Takao; Koguchi, Motoji; Kobayashi, Hiroko; Fujimori, Tohru; Yamatsu, Isao
CORPORATE SOURCE: Dep. Cardiovasc. Dis. Res., Eisai Tsukuba Res. Lab., Tsukuba, 300-26, Japan
SOURCE: Japanese Journal of Pharmacology (1993), 61(1), 7-12
CODEN: JJPAAZ; ISSN: 0021-5198
DOCUMENT TYPE: Journal
LANGUAGE: English
AB E5510, 4-cyano-5,5-bis(4-methoxyphenyl)-4-pentenoic acid, is a new anti-platelet-aggregation agent under development. The authors examined the inhibitory efficacy of E5510 on PDGF-release from washed human platelets. E5510 concentration-dependently inhibited collagen-induced PDGF release from human platelets. PDGF release was reduced to below the detection limit (0.47 ng/mL) by preincubation of platelets with 0.04 μM or higher concns. of E5510. Total growth factor release from platelets was also measured by a bioassay with cultured smooth muscle cells. E5510 almost completely abolished the mitogenic effect of collagen-induced platelet releasates at concns. of 0.04 μM or higher. These data suggest that the release of PDGF and other growth factors was inhibited by E5510 at the same concentration that inhibited platelet aggregation.
IT **111753-73-2**, E5510
RL: BIOL (Biological study)
(platelet-derived growth factor release and human platelet aggregation inhibition by)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



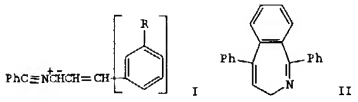
L6 ANSWER 62 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1993:70107 CAPLUS
DOCUMENT NUMBER: 118:70107
TITLE: Electrophotographic photoreceptor
INVENTOR(S): Eto, Yoshihiko; Sakai, Eiichi
PATENT ASSIGNEE(S): Konica Co., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 21 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04242259	A2	19920828	JP 1991-3841	19910117
JP 2961561	B2	19991012		
PRIORITY APPLN. INFO.:			JP 1991-3841	19910117

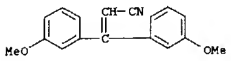
AB In the title photoreceptor comprising an elec. conductive support having thereon a carrier-transporting layer and a carrier-generating layer, the carrier-generating layer contains a p-type carrier-transporting compound and an n-type carrier-transporting compound The title photoreceptor shows high sensitivity.
IT **145498-80-2**
RL: USES (Uses)
(electrophotog. photoreceptor containing)
RN 145498-80-2 CAPLUS
CN Propanedinitrile, [(4-methoxyphenyl)(4-nitrophenyl)methylene]- (9CI) (CA INDEX NAME)



L6 ANSWER 63 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:651232 CAPLUS
DOCUMENT NUMBER: 117:251232
TITLE: Electrocyclic aromatic substitution by nitrile ylides to give 3H-2-benzazepines: substituent effects and mechanism
AUTHOR(S): Groundwater, Paul W.; Sharp, John T.
CORPORATE SOURCE: Dep. Chem., Univ. Edinburgh, Edinburgh, EH9 3JJ, UK
SOURCE: Tetrahedron (1992), 48(37), 7951-64
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:251232
GI



AB Benzonitrile 3,3-diarylallyl ylides I (R = H, Me, OMe, Cl, CF3), generated by the base-induced dehydrochlorination of imidoyl chlorides, cyclized by 1,7-ring closure to give 3H-2-benzazepines e.g., II, in contrast to analogous diazo-compds. which prefer 1,5-electrocyclization. Asym. placed substituents [R in I] favor substitution at the ortho (2') position irresp. of their polar electronic effects. Deuterium labeling studies have shown that the cyclization step is irreversible for these nitrile ylides in contrast to the analogous diazo-compds., for which it is reversible.
IT **144617-66-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and sequential reduction and N-benzoylation of)
RN 144617-66-3 CAPLUS
CN 2-Propenenitrile, 3,3-bis(3-methoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 64 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:531196 CAPLUS
DOCUMENT NUMBER: 117:131196
TITLE: Preparation of (methylimidazopyridymethyl)benzenesulfonamides and related compounds as PAF antagonists
INVENTOR(S): Whittaker, Mark; Miller, Andrew
PATENT ASSIGNEE(S): British Bio-Technology Ltd., UK
SOURCE: PCT Int. Appl., 120 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

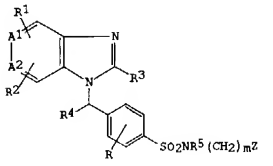
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9203422	A1	19920305	WO 1991-GB1391	19910815
W: AU, CA, FI, HU, JP, KR, NO, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
CA 2088742	AA	19920216	CA 1991-2088742	19910815
CA 2088742	C	20020212		
AU 9184216	A1	19920317	AU 1991-84216	19910815
AU 657920	B2	19950330		
US 5200412	A	19930406	US 1991-745471	19910815
ZA 9106467	A	19930428	ZA 1991-6467	19910815
ZA 9106468	A	19930428	ZA 1991-6468	19910815
EP 543861	A1	19930602	EP 1991-914362	19910815
EP 543861	B1	19981014		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 06500085	T2	19940106	JP 1991-513675	19910815
JP 3218243	B2	20011015		
HU 65983	A2	19940829	HU 1993-390	19910815
AT 172195	E	19981015	AT 1991-914362	19910815
ES 2123511	T3	19990116	ES 1991-914362	19910815
US 5274094	A	19931228	US 1992-992269	19921214
US 5276153	A	19940104	US 1992-990273	19921214
NO 9300499	A	19930414	NO 1993-499	19930212
US 5451676	A	19950919	US 1993-146302	19931101
NO 9703981	A	19930414	NO 1997-3981	19970829
JP 11315070	A2	19991116	JP 1999-94507	19990401
JP 3120075	B2	20001225		

PRIORITY APPLN. INFO.:

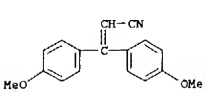
GB 1990-17878	A	19900815
GB 1990-18040	A	19900816
GB 1991-12857	A	19910614
GB 1991-12214	A	19910606
JP 1991-513676	A3	19910815
US 1991-745471	A1	19910815
US 1991-746246	A1	19910815
WO 1991-GB1391	A	19910815
US 1992-992269	A1	19921214

OTHER SOURCE(S): MARPAT 117:131196
GI

L6 ANSWER 64 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



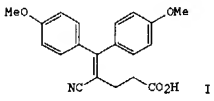
AB Title compds. I [A1 = N,CH,CR1; A2 = N, CH, CR2; both A1 and A2 ≠ N; R = C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, halo, C1-6 alkoxy; R1,R2 = H, C1-6 alkyl, halo, cyano, CO2H, CONH2, CHO, CH2OH, CF3, C1-6 alkoxy, etc.; or R1R2 = atoms to complete a fused Ph ring; R3 = H, C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C1-6 alkoxy, C1-6 alkylthio, CF3, C3-8 cycloalkyl, etc.; R4 = H, (substituted) C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, C2-7 alkanoyl, C1-6 alkylthio, (substituted) Ph, etc.; R5 = H, C1-6 alkyl, C2-6 alkyl, C2-6 alkynyl, C2-7 alkanoyl, (substituted) Ph, C3-8 cycloalkyl, etc.; m = 0-3; Z = CR6R7R8, CR6:CR7R8; R6-R8 = H, halo, (substituted) C1-18 alkyl, C2-18 alkenyl, substituted C1-18 alkoxy, substituted C1-18 alkylthio, C3-8 cycloalkyl, etc.] were prepared as platelet-activating factor (PAF) antagonists useful as antihypotensives and bronchodilators. Thus, 2-methylimidazo[4,5-c]pyridine was N-alkylated by N-1,2-diphenylethyl-4-bromomethylbenzenesulfonamide (preparation given) to give
title compound I [A2 = CH; A1 = N; R, R1, R4, R5 = H; R2 = H; R3 = Me; Z = CHPhCH2Ph; m = 0] (II) and its regioisomer. II had IC50 of 8 nM vs. 3H-PAF receptor binding and in vivo ED50 of 3.1 μg/kg i.v. against PAF-induced hypotension in rats.
IT **101441-96-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for platelet-activating factor antagonists)
RN 101441-96-7 CAPLUS
CN 2-Propenenitrile, 3,3-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 65 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:504432 CAPLUS
DOCUMENT NUMBER: 117:104432
TITLE: Comparative affinity of steroidal and nonsteroidal antiestrogens, cholesterol derivatives and compounds with a dialkylamino side chain for the rat liver antiestrogen binding site
AUTHOR(S): Van den Koedijk, C. D. M. A.; Vis Van Heemst, C.; Elsendoorn, G. M.; Thijssen, J. H. H.; Blankenstein, M. A.
CORPORATE SOURCE: Dep. Pharm., Utrecht Univ., Utrecht, Neth.
SOURCE: Biochemical Pharmacology (1992), 43(12), 2511-18
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Steroidal and non-steroidal antiestrogens, steroidal compds. with (disubstituted) dialkyl amino side chain, cholesterol derivs., and histaminic and (anti)-progestational compds. were tested for their ability to compete with [3H]tamoxifen for the specific antiestrogen binding site (AEBS) in the post-mitochondrial fraction of rat liver homogenates. Relative binding affinity was highest for compds. with diethylamino or pyrrolidino ethoxy side chains. Affinity decreased with shortening of this side chain. No connection could be established between the carbon backbone of the compound and affinity, except for the presence of (sometimes aromatic) ring structures. Steroidal ring structures do not seem to be necessary for binding. The cholesterol derivs. showed very little affinity for the rat liver AEBS. Histamine, melatonin, and the (anti)-progestational compds. showed no affinity for the AEBS; evidently, the AEBS is not identical to receptors for these compds.
IT **143110-72-9**
RL: PRP (Properties)
(antiestrogen binding site affinity of, mol. structure in relation to)
RN 143110-72-9 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(dimethylamino)ethoxy]phenyl]phenylmethylene]-, (Z)- (9CI) (CA INDEX NAME)

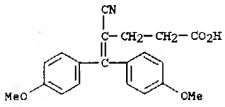
Double bond geometry as shown.

L6 ANSWER 66 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:165596 CAPLUS
DOCUMENT NUMBER: 116:165596
TITLE: E5510, a novel antiplatelet drug with multiple modes of action
AUTHOR(S): Fujimori, Tohru; Harada, Koukichi; Saeki, Takao; Kogushi, Motoji; Katayama, Kouichi; Satoh, Masamichi
CORPORATE SOURCE: Eisai Res. Lab., Eisai Co., Ltd., Tsukuba, Japan
SOURCE: Cardiovascular Drug Reviews (1991), 9(3), 264-84
CODEN: CDREEA; ISSN: 0897-5957
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
GI



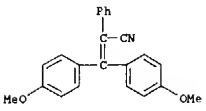
I

AB A review with 55 refs. discussing the mode of action of the novel antiplatelet drug E5510 (I).
IT **111753-73-2**, E5510
RL: BIOL (Biological study)
(antiplatelet activity of, antithrombotic activity in relation to, mechanism of)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



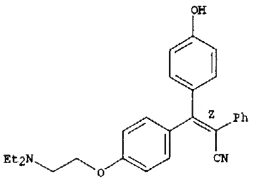
L6 ANSWER 67 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:76526 CAPLUS
DOCUMENT NUMBER: 116:76526
TITLE: Multivariate analysis by the minimum spanning tree method of the structural determinants of diphenylethylenes and triphenylacrylonitriles implicated in estrogen receptor binding, protein kinase C activity, and MCF7 cell proliferation
AUTHOR(S): Dore, Jean Christophe; Gilbert, Jacques; Bignon, Eric; Crastes de Paulet, Andre; Ojasoo, Tiiu; Pons, Michel; Raynaud, Jean Pierre; Miquel, Jean Francois
CORPORATE SOURCE: Mus. Natl. Hist. Nat., Paris, 75005, Fr.
SOURCE: Journal of Medicinal Chemistry (1992), 35(3), 573-83
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The response profiles of 36 para-substituted diphenylethylenes (DPEs) and triphenylacrylonitriles (TPEs) have been compared by multivariate anal. The responses measured were (a) relative binding affinity (RBA) for the cytosol estrogen receptor (ER), (b) ability to promote the growth of the human MCF breast cancer cell-line, (c) cytotoxicity in MCF cells, and (d) ability to stimulate or inhibit protein kinase C (PKC) III activity under 3 different conditions of enzyme activation. The prime object of the anal. was to observe the simultaneous influence of diverse combinations of substituents on all these in vitro responses. To do this, the min. spanning tree (MST) method was used to organize the mols. into a network in which proximate mols. are closely related with regard to their responses whereas remote mols. are distinct. The MST of this population of mols. had 4 main branches. E2 and its TPE mime were located in a central position within the trunk whereas the tips of the branches tended toward mols. of different specificity, i.e., cytotoxic mols. that bind to ER and interfere with PKC, noncytotoxic mols. that also bind to ER and interfere with PKC but promote cell growth, mols. only active on PKC, and mols. active on all parameters except PKC stimulation. A parallel MST anal. of the relations among the response parameters themselves confirmed previous conclusions: For this population of mols., RBAs for ER are fairly closely related to their ability to promote MCF cell growth and only little to cytotoxicity (Bignon, E., et al., 1989). Cytotoxicity is much more clearly correlated with inhibition of diacylglycerol-stimulated PKC activity than with RBAs for ER. PKC inhibition differs substantially depending upon whether the substrate is H, histone, or protamine sulfate.
IT **66422-13-7 104575-13-5 104575-22-6 118976-10-6 118976-11-7 118976-12-8 118976-13-9 118976-14-0 137743-23-8 137743-26-1**
RL: BIOL (Biological study)
(estrogen receptor binding and human breast cancer proliferation and protein kinase C activity response to, mol. structure in relation to)
RN 66422-13-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 67 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



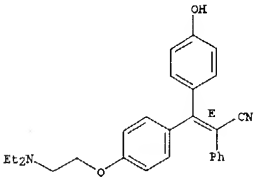
RN 104575-13-5 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 104575-22-6 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

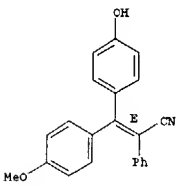
Double bond geometry as shown.



RN 118976-10-6 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)(4-methoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

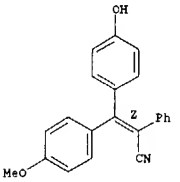
Double bond geometry as shown.

L6 ANSWER 67 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



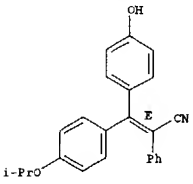
RN 118976-11-7 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)(4-methoxyphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 118976-12-8 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)[4-(1-methylethoxy)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

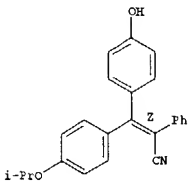
Double bond geometry as shown.



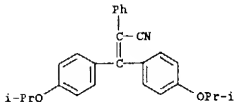
RN 118976-13-9 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)[4-(1-

L6 ANSWER 67 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
methylethoxy)phenyl]methylene]-, (Z)- (9CI) (CA INDEX NAME)

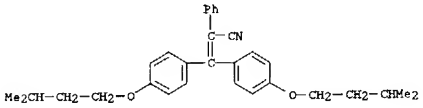
Double bond geometry as shown.



RN 118976-14-0 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-(1-methylethoxy)phenyl]methylene]- (9CI) (CA INDEX NAME)

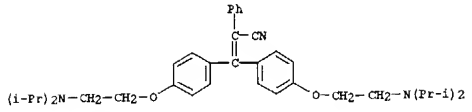


RN 137743-23-8 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-(3-methylbutoxy)phenyl]methylene]- (9CI) (CA INDEX NAME)

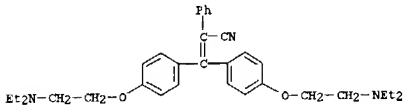


RN 137743-26-1 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-[2-[bis(1-methylethyl)amino]ethoxy]phenyl]methylene]- (9CI) (CA INDEX NAME)

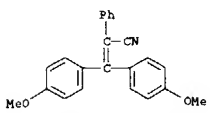
L6 ANSWER 67 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



IT **118976-15-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and estrogen receptor binding and human breast cancer proliferation and protein kinase C activity response to)
RN 118976-15-1 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-[2-(diethylamino)ethoxy]phenyl]methylene]- (9CI) (CA INDEX NAME)



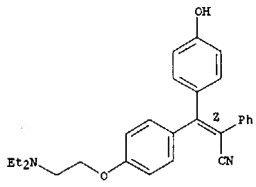
L6 ANSWER 68 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1992:15926 CAPLUS
DOCUMENT NUMBER: 116:15926
TITLE: Influence of di- and tri-phenylethylene estrogen/antiestrogen structure on the mechanisms of protein kinase C inhibition and activation as revealed by a multivariate analysis
AUTHOR(S): Bignon, Eric; Pons, Michel; Dore, Jean Christophe; Gilbert, Jacques; Ojasoo, Tiiu; Miquel, Jean Francois; Raynaud, Jean Pierre; Crastes de Paulet, Andre
CORPORATE SOURCE: INSERM Unite 58, Montpellier, 34090, Fr.
SOURCE: Biochemical Pharmacology (1991), 42(7), 1373-83
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The interaction of 36 di- and tri-phenylethylene derivs. (DPEs and TPEs) with protein kinase C (PKC) was systematically studied. The results were submitted to a multivariate anal. in order to identify the structural features that might be implicated in interference with the activity of 3 PKC subspecies under 3 enzyme activation conditions. Four groups of test-compds., each with common chemical features, could be distinguished clearly. The first group comprised all TPEs substituted with at least one basic dialkylamincethoxy side-chain. These inhibited type α, β, and γ PKC subspecies activated by Ca2+ and phosphatidylserine (PS) with or without diolein (DO) at micromolar concns, but did not inhibit protamine sulfate phosphorylation. The other effectors, which all possessed a 1,1-bis(p-hydroxyphenyl)ethylene moiety, influenced PKC activity at high concns. (30-200 μM) and could be divided into 2 groups. One group constituted PKC inhibitors in the TPE series and inhibited PKC activated by Ca2+, PS and DO, as well as protamine sulfate phosphorylation. The other group constituted dual-type inhibitors/activators in the DPE series and stimulated PKC in the presence of Ca2+ and low PS concns. but inhibited the enzyme in the simultaneous presence of DO. The fourth group of compds. was inactivate and had, for the most part, one or two substituents with weak steric hindrance. In agreement with previous data for six lead compds., this study suggests that, in these chemical series, a basic amino side-chain leads to interaction
with phospholipid and the regulatory domain of PKC, whereas a 1,1-bis(p-hydroxyphenyl)ethylene moiety leads to interaction with the catalytic domain of the enzyme.
IT **66422-13-7 104575-13-5 104575-22-6 118976-12-8 118976-13-9 118976-15-1 137743-23-8 137743-26-1**
RL: BIOL (Biological study)
(protein kinase C response to, mol. structure in relation to)
RN 66422-13-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



RN 104575-13-5 CAPLUS

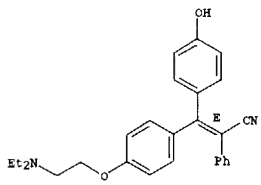
L6 ANSWER 68 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 104575-22-6 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

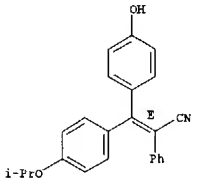
Double bond geometry as shown.



RN 118976-12-8 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)[4-(1-methylethoxy)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

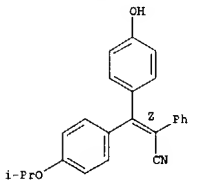
Double bond geometry as shown.

L6 ANSWER 68 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

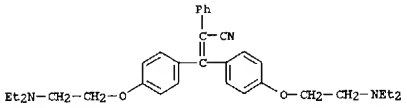


RN 118976-13-9 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)[4-(1-methylethoxy)phenyl]methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

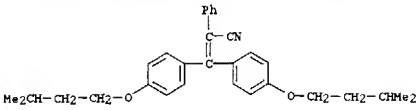


RN 118976-15-1 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-[2-(diethylamino)ethoxy]phenyl]methylene]- (9CI) (CA INDEX NAME)

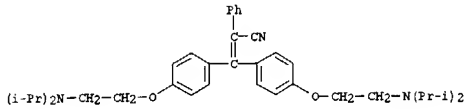


RN 137743-23-8 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-(3-methylbutoxy)phenyl]methylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 68 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 137743-26-1 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-[2-[bis(1-methylethyl)amino]ethoxy]phenyl]methylene]- (9CI) (CA INDEX NAME)



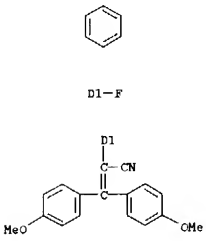
L6 ANSWER 69 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:647458 CAPLUS
DOCUMENT NUMBER: 115:247458
TITLE: Novel prostaglandin synthetase inhibitors
AUTHOR(S): Wu, Taiwen; Ding, Weipei; Si, Yuanzhen; Wu, Xirui
CORPORATE SOURCE: Fac. Pharm., Tongji Med. Univ., Wuhan, Peop. Rep. China
SOURCE: Tongji Yike Daxue Xuebao (1991), 20(2), 77-80
CODEN: TYDXEP; ISSN: 0258-2090
DOCUMENT TYPE: Journal
LANGUAGE: Chinese

AB Sixteen triphenylacrylonitriles (TPA) or diphenylacetylonitriles (DPA) were synthesized by condensing various benzophenones or benzaldehydes with various phenylacetonitriles. The pharmacol. potency of these compds. were studied by the incubation of bovine seminal vesicle microsomes and PG-RIA. The results show that the potency of inhibition of PG biosynthetase of DPA was stronger than that of TPA. Compds. with electron-releasing function groups proved to be more effective than those with electron-attracting function groups. The compound MeO-p-C6H4CH:C(CN)C6H4-p-OMe was the most active one, the potency of which was 40 times stronger than that of naproxen. The structure of some compds. has been analyzed by x-ray diffraction. In addition, the relationship between structure and activity was also investigated by means of x-ray diffraction, UV, and NMR.

IT **131746-45-7P 132029-58-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and prostaglandin synthetase-inhibiting activity of, structure in relation to)

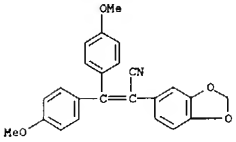
RN 131746-45-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-ar-fluoro- (9CI) (CA INDEX NAME)



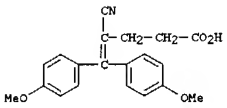
D1—F

RN 132029-58-4 CAPLUS
CN 1,3-Benzodioxole-5-acetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

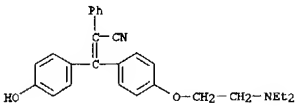
L6 ANSWER 69 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L6 ANSWER 70 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:114849 CAPLUS
DOCUMENT NUMBER: 114:114849
TITLE: A new anti-platelet drug, E5510, has multiple suppressive sites during receptor-mediated signal transduction in human platelets
AUTHOR(S): Fujimori, Tohru; Harada, Koukichi; Saeki, Takao; Kogushi, Motoji; Yoshimura, Tsutomu; Katayama, Kouichi
CORPORATE SOURCE: Eisai Res. Lab., Eisai Co., Ltd., Tsukuba, 300-26, Japan
SOURCE: Japanese Journal of Pharmacology (1991), 55(1), 81-91
CODEN: JJPAAZ; ISSN: 0021-5198
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The mode of action of E5510(4-cyano-5,5bis(4-methoxyphenyl)-4-pentenoic acid) was investigated by examining its effects on the biochem. responses in the process of human platelet activation. In a whole-cell system, E5510 inhibited the increased turnover of inositol phospholipids arising from phospholipase C activation, arachidonic acid release from phospholipids by phospholipase A2, mobilization of intracellular free Ca2+, protein kinase C activation, and TXA2 production In a cell-free system, E5510 inhibited cyclooxygenase activity and cAMP-dependent phosphodiesterase activity in a dose-dependent manner. An elevation of cAMP in platelets was also observed at a relatively high concentration of E5510. The receptor-mediated turnover of inositol phospholipids, intracellular Ca2+ increase, arachidonic acid release from phospholipids, and protein kinase C activation might be indirectly inhibited by the increased cAMP level in platelets. TXA2 production in the whole-cell system was very strongly inhibited by E5510, and the IC50 for this effect was 100 times lower than that of direct inhibition of cyclooxygenase in the cell-free system. Although the primary mode of action of E5510 is the inhibition of the cyclooxygenase pathway of pos. signal transduction in platelets, E5510 has another mode of action by increasing platelet cAMP, which can act as a neg. messenger in platelet signal transduction. These multiple sites of action synergistically antagonize the blood platelet cellular activation.
IT **111753-73-2**, E-5510
RL: BIOL (Biological study)
(blood platelet inhibition by, biochem. mechanism of, in human)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

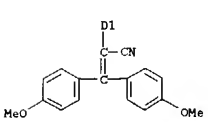


L6 ANSWER 71 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:97232 CAPLUS
DOCUMENT NUMBER: 114:97232
TITLE: Multiple mechanisms of protein kinase C inhibition by triphenylacrylonitrile antiestrogens
AUTHOR(S): Bignon, Eric; Pons, Michel; Gilbert, Jacques; Nishizuka, Yasutomi
CORPORATE SOURCE: Sch. Med., Kobe Univ., Kobe, 650, Japan
SOURCE: FEBS Letters (1990), 271(1-2), 54-8
CODEN: FEBLAL; ISSN: 0014-5793
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The activation of type I (γ), II (β) and III (α) protein kinase (PKC) subspecies by phosphatidylserine (PS) and diacylglycerol (DAG) was inhibited by micromolar concns. of triphenylacrylonitrile (TPE) antiestrogens. TPE A (with p-hydroxy and p-diethylaminoethoxy groups on the 3- and 3'-Ph rings, resp.) interacted with PS-vesicles as well as with the regulatory domain of PKC, probably at a site different from the Ca2+ and DAG binding sites. The interaction of TPE A with the regulatory domain of enzyme was very slow. Apparently, TPE A does not interact with the catalytic domain of PKC. In contrast, another TPE derivative, TPE B (with a p-hydroxy group on each of the 3 Ph rings) inhibited the enzyme activity in a competitive manner with respect to ATP, suggesting that this TPE interacts with the catalytically active site of the enzyme. It seems likely that various TPE antiestrogen derivs. may exert their inhibitory action on PKC by different mechanisms.
IT **113612-21-8**
RL: BIOL (Biological study)
(protein kinase C inhibition by, mechanism of)
RN 113612-21-8 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]- (9CI) (CA INDEX NAME)



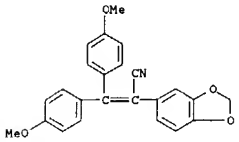
L6 ANSWER 72 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:77536 CAPLUS
DOCUMENT NUMBER: 114:77536
TITLE: New prostaglandin synthetase inhibitors - di- and triphenylacrylonitriles
AUTHOR(S): Ding, Weipei; Wu, Taiwen; Si, Yuanzheng; Wu, Xirui
CORPORATE SOURCE: Fac. Pharm., Tongji Med. Univ., Wuhan, Peop. Rep. China
SOURCE: Journal of Tongji Medical University (1990), 10, 119-23
CODEN: JTMUEI; ISSN: 0257-716X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Sixteen triphenylacrylonitriles (TPE) or diphenylacrylonitriles (DPE) were synthesized by condensation of various benzophenones or benzaldehydes with various phenylacetonitriles. The pharmacol. potency of these compds. was studied by incubation of bovine seminal vesicle microsomes and PG-RIA. The results showed that the potency of inhibition of PG synthetase by DPE was stronger than that by TPE. Compds. with electron-releasing functional groups were more effective than those with electron-attracting groups. Compound DPE-9 was the most active inhibitor, the potency of which was 40-fold stronger than that of naproxen. The structure of some compds. was analyzed by x-ray diffraction. The relation between structure and activity was investigated by means of x-ray diffraction and UV and NMR spectroscopy.
IT **131746-45-7P 132029-58-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and prostaglandin synthetase-inhibiting properties of)
RN 131746-45-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-ar-fluoro- (9CI) (CA INDEX NAME)

D1—F

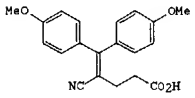


RN 132029-58-4 CAPLUS
CN 1,3-Benzodioxole-5-acetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 72 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



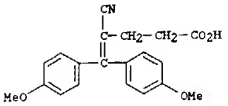
L6 ANSWER 73 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:35693 CAPLUS
DOCUMENT NUMBER: 114:35693
TITLE: Inhibitory effects of a novel antiplatelet aggregating agent, E-5510, on cyclic flow variations in electrically stimulated coronary arteries of the pig
AUTHOR(S): Adachi, Hideyuki; Fujimori, Tohru; Shoji, Tadao
CORPORATE SOURCE: Eisai Tsukuba Res. Lab., Tsukuba, 300-26, Japan
SOURCE: Journal of Cardiovascular Pharmacology (1990), 16(5), 733-41
CODEN: JCPCDT; ISSN: 0160-2446
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

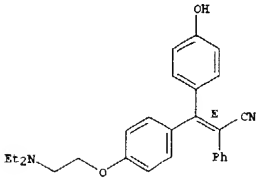
AB The authors examined the inhibitory effects of a novel antiplatelet aggregating agent, E-5510 (I) on cyclic flow variations (CFVs) of coronary blood flow (CBF) in anesthetized open-chest pigs. These CFVs, which are characterized by progressive declines in CBF followed by sudden restoration of flow, were initiated by elec. stimulation of the intimal surface of the left circumflex coronary artery (LCX). A reduction in CBF to zero during CFVs was accompanied by ischemic changes in the surface ECG and regional segment shortening of the left ventricular wall. Occlusive thrombi were detected postmortem in the coronary arteries of the animals in which CFVs had occurred. After CFVs had been observed for 1 h, E-5510 (0.01 or 0.1 mg/kg) or saline was administered i.v. Once CFVs were initiated, both the frequency and the severity (the mean of the three lowest nadirs of CBF) were unchanged by the administration of saline. E-5510 at 0.01 mg/kg decreased the frequency of CFVs from 7.7 to 4.6 CFVs/h and increased the mean lowest nadir from 13.5% of the CBF level before elec. stimulation to 54.3%. E-5510 at 0.1 mg/kg further decreased the frequency from 8.9 to 2.4 CFVs/h, and increased the mean lowest nadir from 14.3% to 53.6%. E-5510, however, showed no ameliorative effect on ischemia-induced myocardial dysfunction, as expressed by the decrease in regional myocardial shortening. Collagen-induced platelet aggregation was significantly inhibited in the platelet-rich plasma of the blood taken at 15 and 60 min after the administration of either dose of E-5510. These results indicate that E-5510 had a potent antiplatelet aggregating effect in this in vivo model, and suggest its potential benefits in treating coronary artery thrombosis.
IT **111753-73-2**, E-5510
RL: BIOL (Biological study)
(coronary circulation and platelet aggregation inhibition by)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 73 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

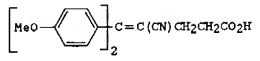


L6 ANSWER 74 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1991:4105 CAPLUS
DOCUMENT NUMBER: 114:4105
TITLE: Protein kinase C subspecies in estrogen receptor-positive and -negative human breast cancer cell lines
AUTHOR(S): Bignon, Eric; Ogita, Kouji; Kishimoto, Akira; Nishizuka, Yasutomi
CORPORATE SOURCE: Sch. Med., Kobe Univ., Kobe, 650, Japan
SOURCE: Biochemical and Biophysical Research Communications (1990), 171(3), 1071-8
CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Estrogen receptor-pos. (MCF7) and -neg. (BT20) human breast cancer cell lines, which are frequently used for studies on cancer chemotherapy with triphenylethylene (TPE) antiestrogens, express at least three protein kinase C subspecies. Two of them are identified as type II PKC having the β-sequence and type III PKC having the α-sequence. The other one shows typical characteristics of PKC which responds to Ca2+, phosphatidylserine and diacylglycerol, but shows kinetic properties subtly different from the previously known PKC subspecies. Immunoblot anal. has shown that this enzyme does not correspond to any of the well defined subspecies with known sequence structures. All of these PKC subspecies are similarly susceptible to the TPE antiestrogens.
IT **104575-22-6**
RL: BIOL (Biological study)
(protein kinase C subspecies inhibition by, of breast cancer cell lines of humans)
RN 104575-22-6 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

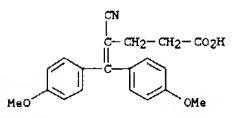


L6 ANSWER 75 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1990:508611 CAPLUS
DOCUMENT NUMBER: 113:108611
TITLE: Determination of 4-cyano-5,5-bis (4-methoxyphenyl)-4-pentenoic acid in human plasma and platelets by gas chromatography-mass spectrometry
AUTHOR(S): Yamano, Yoshiaki; Nakai, Hiromu; Ogawa, Tadasu; Kanazawa, Tamotsu; Morishita, Nobumichi; Yamada, Kouji; Yamagishi, Youji
CORPORATE SOURCE: Tokyo Res. Lab., Eisai Co., Ltd., Tokyo, 112, Japan
SOURCE: Journal of Chromatography (1990), 528(1), 199-207
CODEN: JOCRAM; ISSN: 0021-9673
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB 4-Cyano-5,5-bis(4-methoxyphenyl)-4-pentenoic acid (E5510, I) is a new potential platelet aggregation inhibitor. Solid-phase extraction of drugs combined with gas chromatog.-neg.-ion chemical ionization mass spectrometry (GC-NICI-MS) is a proven sensitive and specific anal. methods for the determination of drugs at low levels in biol. fluids. Prostaglandins in plasma have been quantified with high sensitivity by GC-NICI-MS anal. of the pentafluorobenzyl (PFB) derivs. For example the limit of detection of Iloprost, a stable prostaglandin analog, was 5 pg/mL. A method of determining the PFB derivative of I in plasma and platelets by GC-MS in the NICI mode was developed, and I levels in plasma and platelets after oral administration were determined The high sensitivity of GC-NICI-MS is very attractive since it enables minute amts. of I in platelets to be analyzed. The disposable Bond Elut NH2 columns, which feature both ion-exchange and adsorption, were very efficient for the purification of biol. fluids. By means of this technique, I in human plasma and platelets was sufficiently purified for chromatog. by GC-MS.
IT **111753-73-2**, E5510
RL: ANT (Analyte); ANST (Analytical study)
(determination of, by GC-mass spectrometry, in human blood plasma and platelet)
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 75 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

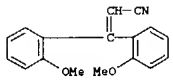
L6 ANSWER 76 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:632526 CAPLUS
DOCUMENT NUMBER: 111:232526
TITLE: Pentadienyl carboxamide derivatives as antagonists of platelet activating factor
AUTHOR(S): Guthrie, Robert W.; Kaplan, Gerald L.; Mennona, Francis A.; Tilley, Jefferson W.; Kierstead, Richard W.; Mullin, John G.; LeMahieu, Ronald A.; Zawoiski, Sonja; O'Donnell, Margaret; et al.
CORPORATE SOURCE: Roche Res. Cent., Hoffmann La Roche Inc., Nutley, NJ, 07110, USA
SOURCE: Journal of Medicinal Chemistry (1989), 32(8), 1820-35
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:232526

AB A series of N-[4-(3-pyridinyl)butyl]-5,5-disubstituted-pentadienamides were prepared by acylation of appropriate amines with diphenylalkenoic acids and evaluated for platelet activating factor (PAF) antagonist activity. Compds. were assayed in vitro in a PAF-binding assay employing washed, whole dog platelets as the receptor source and in vivo after i.v. or oral administration for their ability to prevent PAF-induced bronchoconstriction in guinea pigs. Criteria required for good oral activity in the latter model include: an (E,E)-5-phenyl-2,4-pentadienamide, a second Ph or a four- or five-carbon alkyl moiety in the 5-position of the diene, and an (R)-[1-alkyl-4-(3-pyridinyl)butyl] substituent on the carboxamide nitrogen atom. The alkyl substituent on this side chain can be Me, Et, or cyclopropyl. Two members of this series, [R-(E)]-5,5-bis(4-methoxyphenyl)-N-[1-methyl-4-(3-pyridinyl)butyl]-2,4-pentadienamide (I) and [R-(E,E)]-5-(4-methoxyphenyl)-N-[1-methyl-4-(3-pyridinyl)butyl]-2,4-decadienamide (II) were selected for further pharmacol. evaluation. Both were found to be substantially longer acting after oral administration than the corresponding S enantiomers in the guinea pig bronchoconstriction assay. A second in vivo model used to evaluate PAF antagonists dets. the ability of test compds. to decrease the area of skin wheals induced by an intradermal injection of PAF. In this model, using both rats and guinea pigs, compds. I and II were as active as the reference PAF antagonist 3-[4-(2-chlorophenyl)-9-methyl-6H-thieno[3,2-f][1,2,4]triazolo[4,3-a][1,4]diazepine-2-yl]-1-(4-morpholinyl)-1-propanone.

IT **120553-99-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 120553-99-3 CAPLUS
CN 2-Propenenitrile, 3,3-bis(2-methoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 77 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:624817 CAPLUS
DOCUMENT NUMBER: 111:224817
TITLE: Modes of inhibition of protein kinase C by triphenylacrylonitrile antiestrogens
AUTHOR(S): Bignon, Eric; Ogita, Kouji; Kishimoto, Akira; Gilbert, Jacques; Abecassis, Josephine; Miquel, Jean Francois; Nishizuka, Yasutomi
CORPORATE SOURCE: Sch. Med., Kobe Univ., Kobe, 650, Japan
SOURCE: Biochemical and Biophysical Research Communications (1989), 163(3), 1377-83
CODEN: BBRCA9; ISSN: 0006-291X
DOCUMENT TYPE: Journal
LANGUAGE: English
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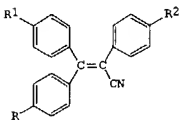
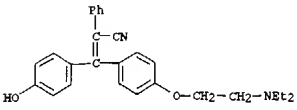


I

AB Protein kinase C (PKC) I (γ), II (β) and III (α) subspecies' activities are inhibited by 3 triphenylacrylonitrile (TPE) antiestrogens at micromolar concns. TPE 1 (I, R = OH; R1 = OCH2CH2NEt2; R2 = H) and TPE 2, I (R = R1 = OCH2CH2NEt2; R2 = H), are competitive with the mechanism of activation by phosphatidylserine (PS). TPE 3, I (R = R1 = R2 = OH), is non-competitive with PS and inhibits the Ca2+- and PS-independent phosphorylation of protamine sulfate by PKC subspecies. This evidence suggests that PKC activity can be inhibited by different routes depending on the TPE structure: TPE 1 and 2 interact with PS as well as with the regulatory domain, whereas TPE 3 inhibits the enzyme by interacting with the catalytically active site.

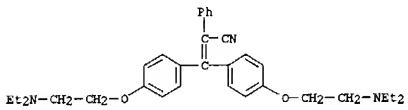
IT **113612-21-8 118976-15-1**
RL: BIOL (Biological study)
(protein kinase C inhibition by, structure in relation to)

RN 113612-21-8 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]- (9CI) (CA INDEX NAME)



RN 118976-15-1 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-[2-(diethylamino)ethoxy]phenyl]methylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 77 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L6 ANSWER 78 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:508482 CAPLUS
DOCUMENT NUMBER: 111:108482
TITLE: Effect of triphenylacrylonitrile derivatives on estradiol-receptor binding and on human breast cancer cell growth
AUTHOR(S): Bignon, Eric; Pons, Michel; Crastes de Paulet, Andre; Dore, Jean Christophe; Gilbert, Jacques; Abecassis, Josephine; Miquel, Jean Francois; Ojasoo, Tiiu; Raynaud, Jean Pierre
CORPORATE SOURCE: INSERM, Montpellier, 34100, Fr.
SOURCE: Journal of Medicinal Chemistry (1989), 32(9), 2092-103
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:108482

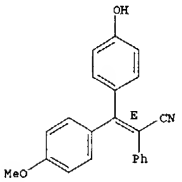
AB In a study of a series of 26 triphenylacrylonitrile derivs., the influence of several possibly interrelated factors on the proliferation of human breast cancer cell lines was studied. The test compds. were for the most part p-hydroxylated with increasingly bulky hydrophobic and(or) basic side chains [isopropyloxy or diethylaminoethoxy] or standard reference compds. The compds. competed diversely with [3H]estradiol binding to calf uterus cytosol and little, if at all, with the binding to the [3H]tamoxifen-labeled antiestrogen binding site in low-speed supernatant. A multiparametric comparison of the relative binding affinities (RBA) recorded for calf, rat, and mouse uterus cytosol estrogen receptor (ER) revealed a possible influence of species-specific receptor conformation and(or) environment on binding. The stimulation and inhibition by these compds. of the proliferation of the ER-pos. human breast cancer cell line MCF7 were measured. Compds. with only hydroxy substituents stimulated proliferation more markedly than methylated derivs. and had a maximum effect at 10-11-10-6M. Stimulation was related to the RBA for the ER. Compds. with isopropyloxy or (diethylamino)ethoxy side chains only weakly stimulated MCF7 cell growth and more powerfully antagonized estradiol-promoted growth. The extent of inhibition depended upon the bulk of the side chain and could be reversed by 10-7M estradiol. Within the same concentration ranges, the test compds. were without an effect on the BT20 ER-neg. cell line. Most of the compds. could arrest the proliferation of both MCF7 and BT20 cells at >3 + 10-6M. This activity was thus independent of the ER. Nevertheless, those compds. with a charged hydrophobic side chain, which were the most powerful antagonists of estradiol-promoted cell growth, were also the most cytotoxic. The overall results for all the mols. on all parameters were submitted to a multivariate anal. (correspondence anal.) which revealed the progressive influence of increasing substitution by hdyroxy and more bulky groups on the generation of antagonist activity and cytotoxicity.

IT **66422-13-7P 104575-13-5P 104575-22-6P**
118976-10-6P 118976-11-7P 118976-12-8P
118976-13-9P 118976-14-0P 118976-15-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and neoplasm inhibition by, in human mammary gland, estrogen receptor antagonism in, structure in relation to)

RN 66422-13-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

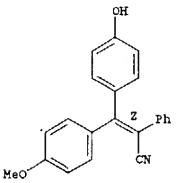
L6 ANSWER 78 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Double bond geometry as shown.



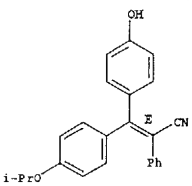
RN 118976-11-7 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)(4-methoxyphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

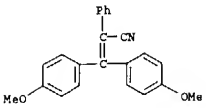


RN 118976-12-8 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)[4-(1-methylethoxy)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

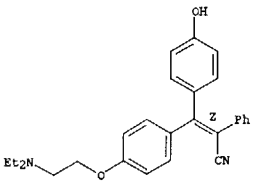


L6 ANSWER 78 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



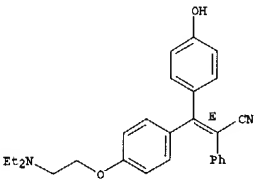
RN 104575-13-5 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 104575-22-6 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

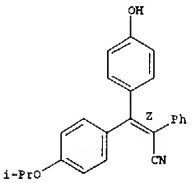
Double bond geometry as shown.



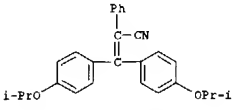
RN 118976-10-6 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)(4-methoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

L6 ANSWER 78 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RN 118976-13-9 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)[4-(1-methylethoxy)phenyl]methylene]-, (Z)- (9CI) (CA INDEX NAME)

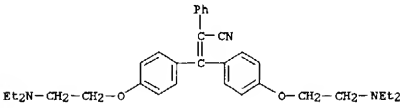
Double bond geometry as shown.



RN 118976-14-0 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-(1-methylethoxy)phenyl]methylene]- (9CI) (CA INDEX NAME)



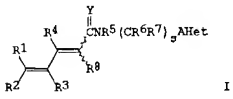
RN 118976-15-1 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-[2-(diethylamino)ethoxy]phenyl]methylene]- (9CI) (CA INDEX NAME)



L6 ANSWER 79 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:212619 CAPLUS
DOCUMENT NUMBER: 110:212619
TITLE: Preparation and formulation of diaryl-N-(pyridinylalkyl)pentadieneamides as platelet activating factor (PAF) antagonists
INVENTOR(S): Guthrie, Robert W.; Kierstead, Richard W.; Tilley, Jefferson W.
PATENT ASSIGNEE(S): Hoffmann-La Roche, Inc., USA
SOURCE: U.S., 69 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4788206	A	19881129	US 1987-72389	19870710
ZA 8804857	A	19890426	ZA 1988-4857	19880706
DK 8803781	A	19890111	DK 1988-3781	19880707
FI 8803290	A	19890111	FI 1988-3290	19880708
NO 8803084	A	19890111	NO 1988-3084	19880708
AU 8818851	A1	19890112	AU 1988-18851	19880708
AU 626526	B2	19920806		
EP 299379	A1	19890118	EP 1988-110934	19880708
EP 299379	B1	19930421		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
HU 48594	A2	19890628	HU 1987-3584	19880708
HU 205902	B	19920728	HU 1988-3584	19880708
AT 88466	E	19930515	AT 1988-110934	19880708
ES 2054740	T3	19940816	ES 1988-110934	19880708
JP 01031766	A2	19890202	JP 1988-171720	19880710
US 4975438	A	19901204	US 1988-241174	19880906
PRIORITY APPLN. INFO.:			US 1987-72389	19870710
			EP 1988-110934	19880708

OTHER SOURCE(S): CASREACT 110:212619; MARPAT 110:212619
GI

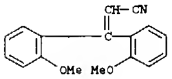


I

AB The title compds. [I; R1, R1 = H, alkyl, cycloalkyl, alkenyl, pyridinyl, (un)substituted Ph, naphthalenyl; R3, R4, R8 = H, alkyl, (un)substituted Ph, naphthalenyl; R5, R6 = H, alkyl; R7 = H, alkyl, cycloalkyl, pyridinylalkyl, (un)substituted Ph, naphthalenyl; Y = O, S; A = p-phenylene, (CH2)nXm(CH2)r; X = O, S, CH:CH; n, r = 0-3; s = 0, 1; m = 0, 1; Het = (un)substituted pyridinyl], their enantiomers, racemates, geometrical isomers, and their pharmaceutically acceptable salts, were prepd. 5,5-Bis(2-methoxyphenyl)-2,4-pentadienoic acid and 4-OZNC6H4CH in CH2Cl2 were treated with dicyclohexylcarbodiimide to give the ester which was condensed with 2-pyridinebutanamine in THF to give (E)-I [A = (CH2)3, R1 = R2 = 2-MeOC6H4, R3-R8 = H, Y = O, Het = 3-pyridinyl, s = 1,] (II). II inhibited PAF with an IC50 of 2 mM. An inhalation aerosol formulation comprised [R-(E,E)]-I [R1 = Me(CH2)3, R2 = 4-MeOC6H4, Y = O, R4-R6 = R8 = H, R7 = Me, A = (CH2)3, Het = 3-pyridinyl] 1, EtOH 30, ascorbic acid 0.5, Freon 12 54.8, and Freon 114 13.7 wt.%.

IT **120553-99-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as platelet activating factor antagonist intermediate)

RN 120553-99-3 CAPLUS
CN 2-Propenenitrile, 3,3-bis(2-methoxyphenyl)- (9CI) (CA INDEX NAME)

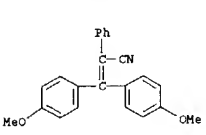


L6 ANSWER 80 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1989:88806 CAPLUS
DOCUMENT NUMBER: 110:88806
TITLE: Analogies and differences in the modulation of progesterone receptor induction and cell proliferation by estrogens and antiestrogens in MCF-7 human breast cancer cells: study with 24 triphenylacrylonitrile derivatives
AUTHOR(S): Bignon, Eric; Pons, Michel; Gilbert, Jacques; Crastes de Paulet, Andre
CORPORATE SOURCE: INSERM, Montpellier, 34090, Fr.
SOURCE: Journal of Steroid Biochemistry (1988), 31(6), 877-85
CODEN: JSTBBK; ISSN: 0022-4731
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Structure-activity relationships in a homogeneous series of 24 triphenylacrylonitrile derivs. were examined with respect to the stimulation of progesterone receptor induction and cell proliferation in MCF-7 cells. In general, triphenylacrylonitrile derivs. were full or partial agonists for both responses; the partial agonists were also able to antagonize the stimulatory action of estradiol. The agonistic activities of the mols. decreased as the size of the lateral side chain increased, but the side-chains correlated with partial agonism of progesterone receptor induction were bulkier than those correlated with partial agonism of cell proliferation. Agonistic and antagonist effects on both responses were correlated with affinity for the estrogen receptor. Half maximal effects on the 2 responses occurred at different concns. (4-fold) of the compds. Thus, in MCF-7 cells, triphenylacrylonitrile modulation of progesterone receptor induction and cell proliferation are mediated by the estrogen receptor; the 2 effects, which occur at different concns. and with slightly different substituents of the compds., are differentially modulated.

IT **66422-13-7 104575-13-5 104575-22-6**
118976-10-6 118976-11-7 118976-12-8
118976-13-9 118976-14-0 118976-15-1
RL: BIOL (Biological study)
(estrogen agonist and antagonist activity of, in breast cancer cell from human, mol. structure in relation to)

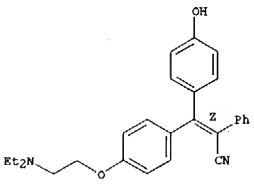
RN 66422-13-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



RN 104575-13-5 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

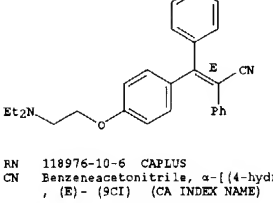
Double bond geometry as shown.

L6 ANSWER 80 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



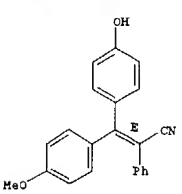
RN 104575-22-6 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 118976-10-6 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)(4-methoxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

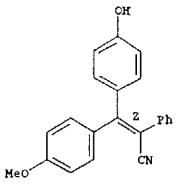
Double bond geometry as shown.



RN 118976-11-7 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)(4-methoxyphenyl)methylene]-

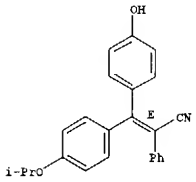
L6 ANSWER 80 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 118976-12-8 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)[4-(1-methylethoxy)phenyl]methylene]-, (E)- (9CI) (CA INDEX NAME)

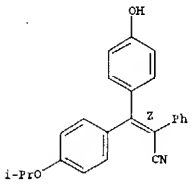
Double bond geometry as shown.



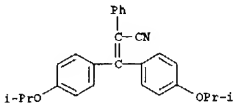
RN 118976-13-9 CAPLUS
CN Benzeneacetonitrile, α-[(4-hydroxyphenyl)[4-(1-methylethoxy)phenyl]methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

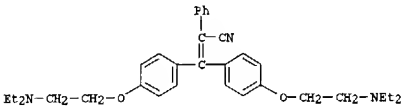
L6 ANSWER 80 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 118976-14-0 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-(1-methylethoxy)phenyl]methylene]- (9CI) (CA INDEX NAME)



RN 118976-15-1 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-[2-(diethylamino)ethoxy]phenyl]methylene]- (9CI) (CA INDEX NAME)



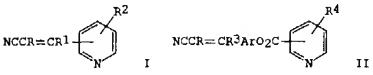
L6 ANSWER 81 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:	1988:580389 CAPLUS
DOCUMENT NUMBER:	109:180389
TITLE:	Electrophotographic photoreceptors containing cyanovinyl group-containing pyridine derivatives
INVENTOR(S):	Matsumoto, Masakazu; Umehara, Masashige; Yoshihara, Yoshiyuki
PATENT ASSIGNEE(S):	Canon K. K., Japan
SOURCE:	Jpn. Kokai Tokkyo Koho, 14 pp. CODEN: JKXXAF
DOCUMENT TYPE:	Patent
LANGUAGE:	Japanese
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63095454	A2	19880426	JP 1986-240656	19861009
JP 07003586	B4	19950118		
PRIORITY APPLN. INFO.:			JP 1986-240656	19861009

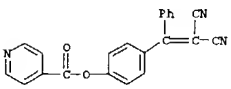
GI



AB The photoconductor layers of the title electrophotog. photoreceptors contain cyanovinyl group-containing pyridine derivs. I or II (R = cyano, alkoxycarbonyl, aryl, heterocyclyl; R1, R2 = H, aryl, heterocyclyl; R2, R4 = H, halo, cyano, NO2, halomethyl; Ar = arylene, heterocyclylene). The photoreceptors show good durability and low residual charge.

IT **116942-01-9 116942-04-2 116942-05-3**
116962-23-3
RL: USES (Uses)
(electrophotog. composite photoconductors containing, for residual potential reduction)

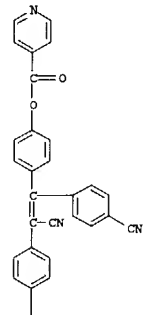
RN 116942-01-9 CAPLUS
CN 4-Pyridinecarboxylic acid, 4-(2,2-dicyano-1-phenylethenyl)phenyl ester (9CI) (CA INDEX NAME)



RN 116942-04-2 CAPLUS
CN 4-Pyridinecarboxylic acid, 4-[2-cyano-1,2-bis(4-cyanophenyl)ethenyl]phenyl ester (9CI) (CA INDEX NAME)

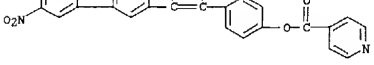
L6 ANSWER 81 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

PAGE 1-A



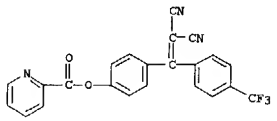
PAGE 2-A

RN 116942-05-3 CAPLUS
CN 4-Pyridinecarboxylic acid, 4-[2-cyano-2-(9-ethyl-6-nitro-9H-carbazol-3-yl)-1-(4-methylphenyl)ethenyl]phenyl ester (9CI) (CA INDEX NAME)



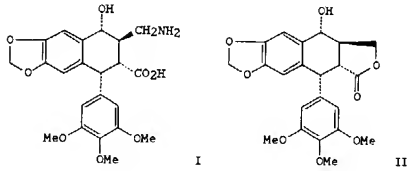
RN 116962-23-3 CAPLUS
CN 2-Pyridinecarboxylic acid, 4-[2,2-dicyano-1-[4-(trifluoromethyl)phenyl]ethenyl]phenyl ester (9CI) (CA INDEX NAME)

L6 ANSWER 81 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L6 ANSWER 82 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:492629 CAPLUS
DOCUMENT NUMBER: 109:92629
TITLE: A highly stereoselective synthesis of podophyllotoxin and analogues based on an intramolecular Diels-Alder reaction
AUTHOR(S): Macdonald, D. I.; Durst, Tony
CORPORATE SOURCE: Ottawa-Carleton Chem. Inst., Univ. Ottawa, Ottawa, ON, K1N 9B4, Can.
SOURCE: Journal of Organic Chemistry (1988), 53(16), 3663-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 109:92629
GI



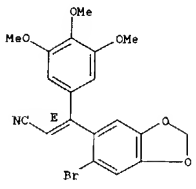
AB trans-2-(3,4,5-Trimethoxyphenyl)-4,5-(methylenedioxy)benzocyclobutenol was coupled with MeO2CCH:CHCH2NCO to yield the urethane, which was hydrolyzed to the acid and heated in MeNO2 to give the tricyclic urethane I. Basic hydrolysis of I generated a γ-amino acid, which was diazotized to yield podophyllotoxin (II). Two analogs of podophyllotoxin were prepared via a similar route.

IT **115140-86-8P 115140-87-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 115140-86-8 CAPLUS
CN 2-Propenenitrile, 3-(6-bromo-1,3-benzodioxol-5-yl)-3-(3,4,5-trimethoxyphenyl)-, (E)- (9CI) (CA INDEX NAME)

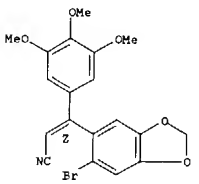
Double bond geometry as shown.

L6 ANSWER 82 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 115140-87-9 CAPLUS
CN 2-Propenenitrile, 3-(6-bromo-1,3-benzodioxol-5-yl)-3-(3,4,5-trimethoxyphenyl)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L6 ANSWER 83 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:473155 CAPLUS
DOCUMENT NUMBER: 109:73155
TITLE: Diphenylmethane derivatives, a procedure for preparing them, pharmaceutical compositions containing them, and their use in treatment of diseases caused by blood stream disorders
INVENTOR(S): Yamagishi, Youji; Akasaka, Kozo; Suzuki, Takeshi; Miyamoto, Mitsuaki; Nakamoto, Kouji; Okano, Kazuo; Abe, Shinya; Ikuta, Hironori; Hayashi, Kenji; et al.
PATENT ASSIGNEE(S): Eisai Co., Ltd., Japan
SOURCE: Eur. Pat. Appl., 36 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

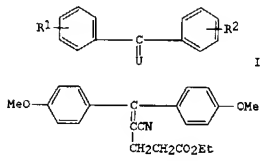
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 238973	A2	19870930	EP 1987-103834	19870317
EP 238973	A3	19891004		
EP 238973	B1	19921202		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 62223164	A2	19871001	JP 1986-65963	19860326
JP 07103082	B4	19951108		
FI 8701022	A	19870918	FI 1987-1022	19870309
FI 92189	B	19940630		
FI 92189	C	19941010		
US 4886834	A	19891212	US 1987-24737	19870311
DK 8701334	A	19870918	DK 1987-1334	19870316
NO 8701072	A	19870918	NO 1987-1072	19870316
NO 168577	B	19911202		
NO 168577	C	19920311		
DD 263233	A5	19881228	DD 1987-300831	19870316
DD 278782	A5	19900516	DD 1987-324890	19870316
DD 278780	A5	19900516	DD 1987-324892	19870316
DD 283373	A5	19901010	DD 1987-324891	19870316
CA 1296338	A1	19920225	CA 1987-532108	19870316
AU 8770085	A1	19870924	AU 1987-70085	19870317
AU 593334	B2	19900208		
CN 87101979	A	19871028	CN 1987-101979	19870317
CN 1014889	B	19911127		
JP 63010743	A2	19880118	JP 1987-60022	19870317
JP 2547207	B2	19961023		
HU 44007	A2	19880128	HU 1987-1156	19870317
HU 196589	B	19881228		
EP 346943	A1	19891220	EP 1989-114183	19870317
EP 346943	B1	19930217		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
EP 478001	A1	19920401	EP 1991-119345	19870317
EP 478001	B1	19960612		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
EP 479332	A2	19920408	EP 1991-119344	19870317
EP 479332	A3	19920415		
EP 479332	B1	19950621		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 82956	E	19921215	AT 1987-103834	19870317
AT 85794	E	19930315	AT 1989-114183	19870317
ES 2043982	T3	19940101	ES 1989-114183	19870317
ES 2052504	T3	19940716	ES 1987-103834	19870317

L6 ANSWER 83 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

ES 2073648	T3	19950816	ES 1991-119344	19870317
AT 139225	E	19960615	AT 1991-119345	19870317
ES 2087950	T3	19960801	ES 1991-119345	19870317
SU 1797606	A3	19930223	SU 1989-4613517	19890227
SU 1715204	A3	19920223	SU 1989-4613563	19890228
US 4954523	A	19900904	US 1989-364712	19890609
US 4978767	A	19901218	US 1989-364710	19890609
US 5034418	A	19910723	US 1989-364711	19890609
US 5064848	A	19911112	US 1990-518816	19900504
US 5206403	A	19930427	US 1990-609374	19901105
US 5103010	A	19920407	US 1990-612829	19901113
US 5182301	A	19930126	US 1991-659518	19910221
RU 2034831	C1	19950510	RU 1992-5010552	19920115
JP 07002726	A2	19950106	JP 1994-21138	19940218
JP 08259441	A2	19961008	JP 1995-336383	19951225
JP 08225508	A2	19960903	JP 1996-7001	19960119
PRIORITY APPLN. INFO.:			JP 1986-57061	19860317
			JP 1986-65963	19860326
			US 1987-24737	19870311
			EP 1987-103834	19870317
			EP 1989-114183	19870317
			US 1989-364710	19890609
			US 1989-364711	19890609
			US 1989-364712	19890609

OTHER SOURCE(S): CASREACT 109:73155

GI



I

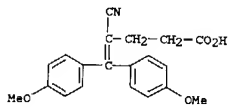
II

AB Diphenylmethane derivs. I [R1, R2 = H, OH, alkoxy; U = :CXY, :NOW; X = H, cyano, COR6; R6 = OH, NH2; Y = R10CO2R3; R3 = H, alkoxy; R10 = alkylene; CONR4R5, R4, R5 = H, alkyl, arylalkyl, CH2NHSO2Ph, CR8:NR7, R7 = alkoxy, aryl, R8 = VR9, V = O, S, N, R9 = alkyl, aryl; W = CH2COCH2CO2R13, R13 = H, alkyl, CH2C(:NOR14)CH2CO2R15, R15 = H, alkyl, R14 = alkyl, CH(CN)(CH2)qCO2R16, R16 = H, alkyl, q = 1-3, (CH2)pZ, Z = SH, SCN, monovalent (un)substituted ring, p = 1, 2], useful in inhibiting agglomeration of blood, were prepared A mixture of 4-MeOC6H4COC6H4OMe-4, Zn, and B(OMe)3 in THF was treated with BrCH(CN)(CH2)2CO2Et and a catalytic amount iodine and the whole kept at room temperature 5 h to give cyanopentenoate II. In guinea pigs the ED50 of inhibiting collagen-induced agglutination of blood was 0.05 mg/kg orally for II.

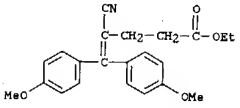
L6 ANSWER 83 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

IT **111753-73-2P 115499-63-3P 115499-64-4P**
115499-78-0P 115499-79-1P 115499-80-4P
115499-82-6P 115499-85-9P 115499-98-4P
115500-00-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as remedy for blood stream disorder diseases)

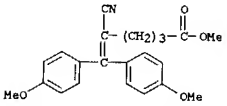
RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 115499-63-3 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

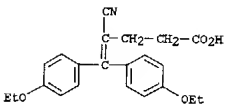


RN 115499-64-4 CAPLUS
CN 5-Hexenoic acid, 5-cyano-6,6-bis(4-methoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)



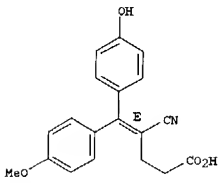
RN 115499-78-0 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-ethoxyphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 83 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



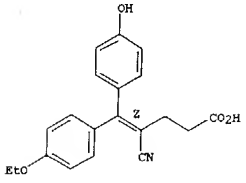
RN 115499-79-1 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5-(4-hydroxyphenyl)-5-(4-methoxyphenyl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



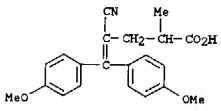
RN 115499-80-4 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5-(4-ethoxyphenyl)-5-(4-hydroxyphenyl)-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

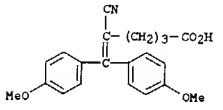


RN 115499-82-6 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)

L6 ANSWER 83 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

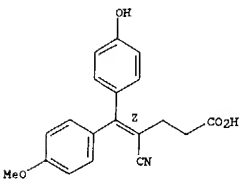


RN 115499-85-9 CAPLUS
CN 5-Hexenoic acid, 5-cyano-6,6-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 115499-98-4 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5-(4-hydroxyphenyl)-5-(4-methoxyphenyl)-, (Z)- (9CI) (CA INDEX NAME)

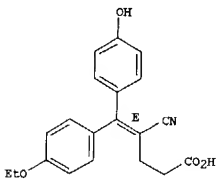
Double bond geometry as shown.



RN 115500-00-0 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5-(4-ethoxyphenyl)-5-(4-hydroxyphenyl)-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L6 ANSWER 83 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



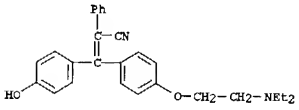
L6 ANSWER 84 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:431629 CAPLUS
DOCUMENT NUMBER: 109:31629
TITLE: Mechanisms of growth inhibition by nonsteroidal antiestrogens in human breast cancer cells
AUTHOR(S): Sutherland, Robert L.; Watts, Colin K. W.; Hall, Rosemary E.; Ruenitz, Peter C.
CORPORATE SOURCE: Garvan Inst. Med. Res., St. Vincent's Hosp., Sydney, 2010, Australia
SOURCE: Journal of Steroid Biochemistry (1987), 27(4-6), 891-7
CODEN: JSTBBK; ISSN: 0022-4731
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Treatment of MCF7 human mammary carcinoma cells with the nonsteroidal antiestrogens, tamoxifen and clomiphene, leads to a concentration-dependent decrease in cellular proliferation rate which can be resolved into estrogen-reversible and estrogen-irreversible components. This became more clearly apparent when cells were treated with the 4-hydroxylated derivs. of these compds. where, because of enhanced affinity for the estrogen receptor (ER), the dose-response curves for the two components could be separated Thus treatment with 4-hydroxyclomiphene resulted in a distinct biphasic effect on cell growth. In the concentration range 10-10-10-8 M, cell proliferation was inhibited in a concentration-dependent manner to a maximum of 60-70%, there was no further effect between 10-8 and 10-6 M, but at concns. >10-6 M there was another concentration-dependent decrease in cell growth. Studies with a series of vinyl-substituted hydroxytriphenylethylenes revealed that in the nanomolar concentration range, where the effects of the drugs could be completely negated by the simultaneous addition of estradiol, the potency for growth inhibition was highly correlated with affinity for ER. Such data provide strong evidence that in this concentration range, the growth inhibitory effects of nonsteroidal antiestrogens are mediated by the intracellular ER. In the micromolar concentration range, the effects of antiestrogens are not completely reversed by estradiol, potency is not well correlated with affinity for either ER or the antiestrogen binding site (AEBS) but the effect is cell cycle phase-specific. Furthermore, the disparity between the affinity for AEBS (0.8-3.3 nM) and the concentration of drug needed for estrogen-irreversible growth inhibition (≥2.5 μM) argue against a central role for AEBS in mediating this effect. The observation that triphenylethylene antiestrogens are calmodulin antagonists may provide some insight into potential mechanisms for this estrogen-irreversible effect. Indeed, in identical expts., two phenothiazine calmodulin antagonists inhibited MCF 7 cell proliferation at concns. ≥2.5 + 10-6 M. Growth inhibition following administration of fluphenazine, perphenazine and triphenylethylene antiestrogens was accompanied by qual. similar changes in the cell cycle kinetic parameters, i.e. accumulation in G1 phase at the expense of S phase cells. These data suggest triphenylethylene antagonism of calmodulin activated cellular processes as a potential mechanism for the estrogen-irreversible effects of the nonsteroidal antiestrogens.

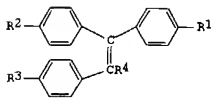
IT **113612-21-8**
RL: BIOL (Biological study)
(mammary gland neoplasm growth inhibition by, of humans, calmodulin

L6 ANSWER 84 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
antagonism and estrogen receptor binding in relation to)
RN 113612-21-8 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]- (9CI) (CA INDEX NAME)



L6 ANSWER 85 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

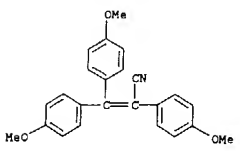
ACCESSION NUMBER: 1988:160932 CAPLUS
DOCUMENT NUMBER: 108:160932
TITLE: Quantitative structure-activity relationship studies on prostaglandin synthetase (PGS) inhibitors
AUTHOR(S): Gupta, S. P.; Prabhakar, Y. S.; Singh, P.
CORPORATE SOURCE: Dep. Chem., Birla Inst. Technol. Sci., Pilani, 333 031, India
SOURCE: Current Science (1987), 56(21), 1090-2
CODEN: CUSCAM; ISSN: 0011-3891
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

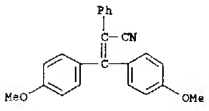
AB The quant. structure-activity relations for prostaglandin synthetase inhibition is described for triphenylacrylonitriles and triphenylethylenes (I, R1 and R2 and R3 = H, OH, Me, OMe, F, Cl, NH2; R4 = H, CN, CH2NH2, CH2NHAc, CONH2). The inhibitory activity was best with I with a CN group and appeared to involve hydrophobic and electronic interactions.

IT **35364-39-7 66422-13-7 82925-22-2**
82925-23-3 82925-24-4 82925-25-5
82925-26-6 84836-18-0 84836-19-1
84836-20-4 84836-21-5 84836-22-6
84836-23-7 84836-24-8 84836-25-9
RL: BIOL (Biological study)
(prostaglandin synthetase inhibition by, electronic interactions and hydrophobicity in)
RN 35364-39-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-4-methoxy- (9CI) (CA INDEX NAME)

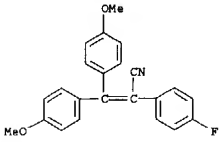


RN 66422-13-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 85 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

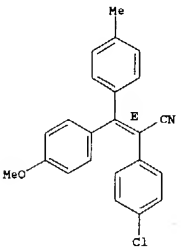


RN 82925-22-2 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-4-fluoro- (9CI) (CA INDEX NAME)



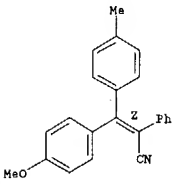
RN 82925-23-3 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



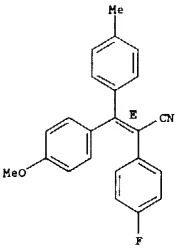
RN 82925-24-4 CAPLUS
CN Benzeneacetonitrile, α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

L6 ANSWER 85 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
Double bond geometry as shown.



RN 82925-25-5 CAPLUS
CN Benzeneacetonitrile, 4-fluoro-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

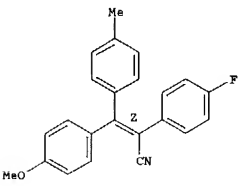
Double bond geometry as shown.



RN 82925-26-6 CAPLUS
CN Benzeneacetonitrile, 4-fluoro-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

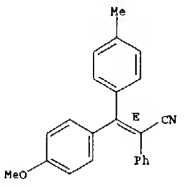
Double bond geometry as shown.

L6 ANSWER 85 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 84836-18-0 CAPLUS
CN Benzeneacetonitrile, α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

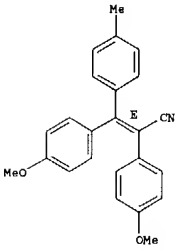
Double bond geometry as shown.



RN 84836-19-1 CAPLUS
CN Benzeneacetonitrile, 4-methoxy-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

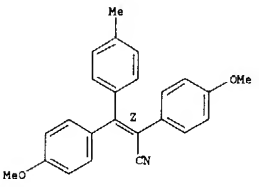
Double bond geometry as shown.

L6 ANSWER 85 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 84836-20-4 CAPLUS
CN Benzeneacetonitrile, 4-methoxy-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

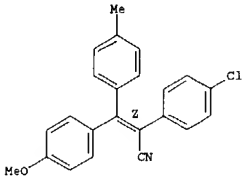
Double bond geometry as shown.



RN 84836-21-5 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

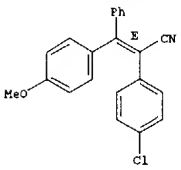
Double bond geometry as shown.

L6 ANSWER 85 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



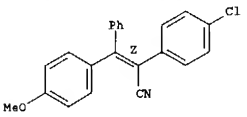
RN 84836-22-6 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[(4-methoxyphenyl)phenylmethylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



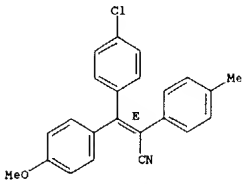
RN 84836-23-7 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[(4-methoxyphenyl)phenylmethylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

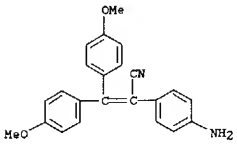


RN 84836-24-8 CAPLUS
CN Benzeneacetonitrile, α-[(4-chlorophenyl)(4-methoxyphenyl)methylene]-4-methyl-, (E)- (9CI) (CA INDEX NAME)

L6 ANSWER 85 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
Double bond geometry as shown.

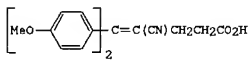


RN 84836-25-9 CAPLUS
CN Benzeneacetonitrile, 4-amino-α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



L6 ANSWER 86 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1988:386 CAPLUS
DOCUMENT NUMBER: 108:386
TITLE: Pharmacological properties of the novel anti-platelet aggregating agent 4-cyano-5,5-bis(4-methoxyphenyl)-4-pentenoic acid
AUTHOR(S): Fujimori, T.; Harada, K.; Saeki, T.; Kogushi, M.; Akasaka, K.; Yamagishi, Y.; Yamatsu, I.
CORPORATE SOURCE: Eisai Res. Lab., Eisai Co., Ltd., Ibaraki, 300-26, Japan
SOURCE: Arzneimittel-Forschung (1987), 37(10), 1143-8
CODEN: ARZNAD; ISSN: 0004-4172
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

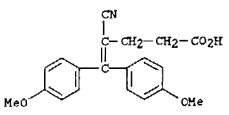


I

AB Various pharmacol. properties of a new antiplatelet aggregating agent, 4-cyano-5,5-bis(4-methoxyphenyl)-4-pentenoic acid (E-5510) (I) were examined. E-5510 inhibited human platelet aggregation induced by collagen, arachidonic acid, ADP, platelet activating factor (PAF) and epinephrine. Thrombin-induced platelet aggregation, which was not inhibited by acetylsalicylic acid (ASA) or the thiazole drug, 4,5-bis(4-methoxyphenyl)-2-(trifluoromethyl)thiazole, was inhibited by E-5510. E-5510 inhibited collagen-induced platelet aggregation in platelet-rich plasma (PRP) from guinea pigs, beagle dogs and monkey to the same degree as in human PRP, but its effect was weaker in rat PRP. Human platelet adhesion to a collagen-coated plastic disk and thrombin-induced ATP release from human platelets were also inhibited by this compound. Next, the ex vivo anti-platelet effect of E-5510 was examined in guinea pigs and beagle dogs. E-5510 was the most potent among the tested drugs (ticlopidine, ASA, cilostazol and the thiazole drug). The anti-platelet effect of this compound appeared within 1 h and laster more than 8 h after oral administration. This compound is a promising candidate as an antithrombotic drug for clin. use. Possible mechanisms of the antiplatelet action of E-5510 are discussed.

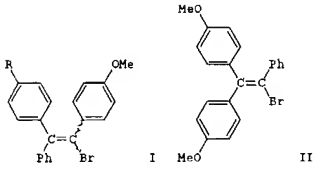
IT **111753-73-2**
RL: BIOL (Biological study)
(antiplatelet aggregating agent, pharmacol. of)

RN 111753-73-2 CAPLUS
CN 4-Pentenoic acid, 4-cyano-5,5-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



L6 ANSWER 87 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:195797 CAPLUS
DOCUMENT NUMBER: 106:195797
TITLE: Ipso substitution by cyanide anion in photolysis of 1-(p-methoxyphenyl)vinyl bromides
AUTHOR(S): Kitamura, Tsugio; Murakami, Mahito; Kobayashi, Shinjiro; Taniguchi, Hiroshi
CORPORATE SOURCE: Fac. Eng., Kyushu Univ., Fukuoka, 812, Japan
SOURCE: Tetrahedron Letters (1986), 27(33), 3885-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:195797
GI

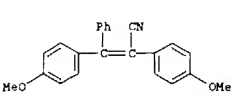


I II

AB Photolysis of 1-(p-methoxyphenyl)vinyl bromides I (R = H, OMe) and II in the presence of cyanide anion provided 1-cyano-1-(p-cyanophenyl)ethylenes and 3,10-dicyanophenanthrenes. These were formed via a vinyl cation.

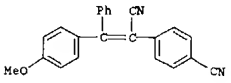
IT **108177-17-9P 108177-18-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 108177-17-9 CAPLUS
CN Benzeneacetonitrile, 4-methoxy-α-[(4-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)



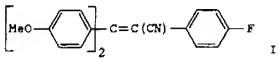
RN 108177-18-0 CAPLUS
CN Benzeneacetonitrile, 4-cyano-α-[(4-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 87 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L6 ANSWER 88 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:113127 CAPLUS
DOCUMENT NUMBER: 106:113127
TITLE: Inhibition of platelet aggregation by novel triphenylethylene analogs
AUTHOR(S): Rao, Gundu H. R.; John, Vargese; Hill, Timothy D.; Vennerstrom, J. L.; White, James G.; Holmes, T. J., Jr.
CORPORATE SOURCE: Health Sci. Cent., Univ. Minnesota, Minneapolis, MN, 55455, USA
SOURCE: Thrombosis Research (1986), 44(4), 527-38
CODEN: THBRAA; ISSN: 0049-3848
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

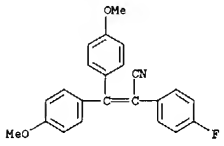


I

AB The effect of 6 newly synthesized triphenylethylene (TPE) analogs on platelet arachidonic acid [506-32-1] metabolism and function was evaluated. All compds. tested inhibited arachidonic acid induced platelet aggregation and several were superior to aspirin in their relative potency. Introduction of a carboxyl function into the α-ring, which should enhance binding according to proposed structural models for cyclooxygenase [39391-18-9] inhibitors, was not found to be beneficial. Increased structural rigidity, which resulted from covalent linkage of two aromatic rings in this series, did not eliminate anti-aggregatory properties. I [**82925-22-2**] was the most potent of the 6 derivs. tested.

IT **82925-22-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and platelet aggregation of human inhibition by)

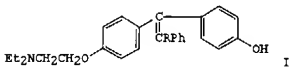
RN 82925-22-2 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-4-fluoro- (9CI) (CA INDEX NAME)



L6 ANSWER 88 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L6 ANSWER 89 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:66833 CAPLUS
DOCUMENT NUMBER: 106:66833
TITLE: Substituted-vinyl hydroxytriarylethylenes, 1-[4-[2-(diethylamino)ethoxy]phenyl]-1-(4-hydroxyphenyl)-2-phenylethylenes: synthesis and effects on MCF 7 breast cancer cell proliferation
AUTHOR(S): Ruenitz, Peter C.; Bagley, Jerome R.; Watts, Colin K. W.; Hall, Rosemary E.; Sutherland, Robert L.
CORPORATE SOURCE: Coll. Pharm., Univ. Georgia, Athens, GA, 30602, USA
SOURCE: Journal of Medicinal Chemistry (1986), 29(12), 2511-19
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:66833
GI



I

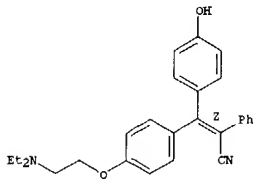
AB Triarylethylene compds. I (R = Et, Br, H, CN, NO2) related to 4-hydroxyclomiphene (I; R = Cl) were synthesized to facilitate studies of the mol. actions of synthetic nonsteroidal antiestrogens. The relative binding affinities of I for the estrogen receptor (ER) and the antiestrogen binding site (AEBS) in MCF 7 human mammary carcinoma cells were measured and correlated with the effects of these drugs on cell proliferation kinetics. Affinities for ER and AEBS were highly correlated, illustrating that vinyl substituents influence binding to ER and AEBS in a parallel manner. The data indicates two distinct mechanisms of growth inhibition by triarylethylene antiestrogens and that among the vinyl substitutions examined to date the Cl substituent yields the most active mol. both in terms of affinity for ER and AEBS and potency as a growth inhibitory agent.

IT **104575-13-5P 104575-22-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cancer cell inhibitory activity)

RN 104575-13-5 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

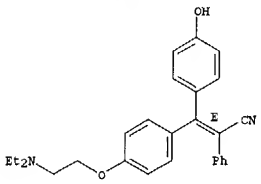
Double bond geometry as shown.

L6 ANSWER 89 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

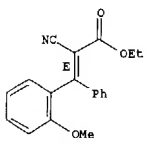


RN 104575-22-6 CAPLUS
CN Benzeneacetonitrile, α-[[4-[2-(diethylamino)ethoxy]phenyl](4-hydroxyphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

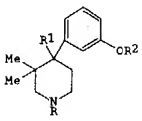
Double bond geometry as shown.



L6 ANSWER 90 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L6 ANSWER 90 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1985:220708 CAPLUS
DOCUMENT NUMBER: 102:220708
TITLE: Synthesis and analgesic properties of 1,3,3,4,4-substituted piperidines
AUTHOR(S): Huegi, B.; Maurer, R.; Roemer, D.; Petcher, T. J.
CORPORATE SOURCE: Praeklin. Forsch., Sandoz A.-G., Basel, CH-4002, Switz.
SOURCE: European Journal of Medicinal Chemistry (1984), 19(6), 487-94
CODEN: EJMCA5; ISSN: 0223-5234
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 102:220708
GI



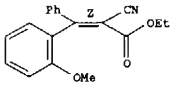
I

AB The title compds. [I; R = CH2:CHCH2, (1-hydroxycyclopropyl)methyl, (un)substituted alkyl, PhCH2CH2; R1 = Me, Ph; R2 = H, Me] were prepared in 8 steps from 3-MeOC6H4CR1:C(CN)CO2Et and tested for analgesic, morphinomimetic and morphine antagonist properties. I (R1 = Me) had no biol. activity. The x-ray crystal structure of I (R = R1 = R2 = Me) was determined

IT **96610-30-9P 96610-31-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, lithiation, and addition reaction of, with Et acetate)

RN 96610-30-9 CAPLUS
CN 2-Propenoic acid, 2-cyano-3-(2-methoxyphenyl)-3-phenyl-, ethyl ester, (Z)- (9CI) (CA INDEX NAME)

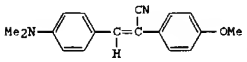
Double bond geometry as shown.



RN 96610-31-0 CAPLUS
CN 2-Propenoic acid, 2-cyano-3-(2-methoxyphenyl)-3-phenyl-, ethyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L6 ANSWER 91 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:416795 CAPLUS
DOCUMENT NUMBER: 101:16795
TITLE: The effect of various acrylonitriles and related compounds on prostaglandin biosynthesis
AUTHOR(S): Michel, F.; Mercklein, L.; De Paulet, A. Crastes; Dore, J. C.; Gilbert, J.; Miquel, J. F.
CORPORATE SOURCE: Lab. Biochim. Steroides, Montpellier, 34100, Fr.
SOURCE: Prostaglandins (1984), 27(1), 69-84
CODEN: PRGLBA; ISSN: 0090-6980
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

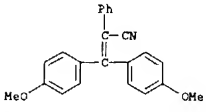


I

AB The effect of nearly 90 arylacrylonitrile derivs., and of several related compds., on the biosynthesis of prostaglandins by bovine seminal vesicle microsomes was studied. This effect was compared to that of triarylacrylonitrile derivs. known for their inhibiting properties. Several arylacrylonitrile derivs. proved to be good inhibitors of prostaglandin synthetase [9055-65-6], especially certain N-trisubstituted compds.: trans-3-(4-dimethylaminophenyl)-2-(4-methoxyphenyl)acrylonitrile (I) [73151-50-5] was the best inhibitor of the group, with a 50% inhibitory concentration of 0.07 μM. Structure-activity relations are discussed.

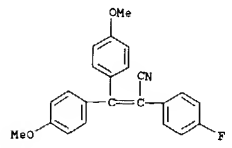
IT **66422-13-7 82925-22-2 89986-16-3**
RL: BIOL (Biological study)
(prostaglandin synthetase inhibition by, structure in relation to)

RN 66422-13-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

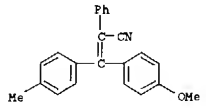


RN 82925-22-2 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-4-fluoro- (9CI) (CA INDEX NAME)

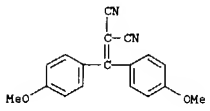
L6 ANSWER 91 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



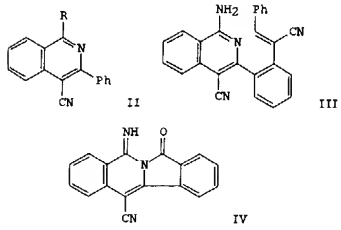
RN 89986-16-3 CAPLUS
CN Benzeneacetonitrile, α-[(4-methoxyphenyl)(4-methylphenyl)methylene]- (9CI) (CA INDEX NAME)



L6 ANSWER 92 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1984:138435 CAPLUS
DOCUMENT NUMBER: 100:138435
TITLE: Mass spectra of dicyanomethylene derivatives of benzophenone analogs
AUTHOR(S): Wang, Ching Bore; Her, Guor Rong; Watson, J. Throck
CORPORATE SOURCE: Dep. Biochem., Michigan State Univ., East Lansing, MI, 48824, USA
SOURCE: Organic Mass Spectrometry (1983), 18(11), 457-61
CODEN: ORMSBG; ISSN: 0030-493X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The dicyanomethylene derivative of a benzophenone analog, e.g. Ph2C:C(CN)2, significantly alters the fragmentation pattern observed during electron impact ionization of the underivatized parent compound A double bond connecting the dicyanomethylene moiety to the parent compound is cleaved during a major fragmentation path for many of these compds. A mechanism involving rearrangement of two H atoms is proposed to explain cleavage of this double bond. Conventional mass spectra as well as collisionally activated dissociation mass spectra of selected ions of several model compds.
are reported in support of a proposed fragmentation mechanism.
IT **21453-19-0P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and mass spectrum of)
RN 21453-19-0 CAPLUS
CN Propanedinitrile, [bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

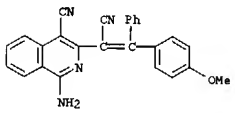


L6 ANSWER 93 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1983:612404 CAPLUS
DOCUMENT NUMBER: 99:212404
TITLE: Heterocyclic imines and amines. Part 19. Isoquinoline and other products from α,o-dicyanostilbene and basic reagents
AUTHOR(S): Barnard, Ian F.; Elvidge, John A.
CORPORATE SOURCE: Chem. Dep., Univ. Surrey, Guildford, GU2 5XH, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1983), (8), 1813-18
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 99:212404
GI

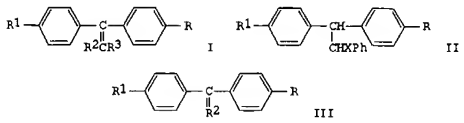


AB 2-NCC6H4C(CN):CHPh (I) was cleaved by N2H4 or NH2OH under mildly acidic conditions to give 2-NCC6H4CH2CN and PhCHO, isolated as derivs. Reactions of I with NaNH2 and with NaOR (R = Me, Et, Pr, Bu) gave the corresponding isoquinolines II (R = NH2, OMe, OEt, OPr, OBu); the intermediate 3,4-dihydroisoquinoline in the reaction with NaOMe was isolated and gave II (R = OMe) on dehydrogenation. Acid hydrolysis of II (R = OEt) gave 4-cyano-3-phenylisoquinolin-1(2H)-one. Reaction of I with 2-NCC6H4CH2CN in MeOH containing NaOMe at 60° for 4 h gave amine III which on oxidation followed by dehydration gave isoindoloisoquinolinone IV.
IT **87895-31-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 87895-31-6 CAPLUS
CN 3-Isoquinolineacetonitrile, 1-amino-4-cyano-α-[(4-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 93 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

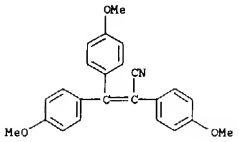


L6 ANSWER 94 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1983:154902 CAPLUS
DOCUMENT NUMBER: 98:154902
TITLE: Inhibition of prostaglandin synthetase by di- and triphenylethylene derivatives: a structure-activity study
AUTHOR(S): Gilbert, Jacques; Miquel, Jean Francois; Precigoux, Gilles; Hospital, Michel; Raynaud, Jean Pierre; Michel, Francoise; Crastes de Paulet, Andre
CORPORATE SOURCE: Cent. Etudes Rech. Chim. Org. Appl., CNRS, Thiais, 94320, Fr.
SOURCE: Journal of Medicinal Chemistry (1983), 26(5), 693-9
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

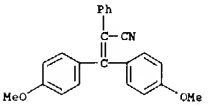


AB The title compds. I (R = H, F, OH, Me, MeO, AcO; R1 = H, Cl, F, OH, Me, MeO, AcO; R2 = Et, CHMe2 CMe3, Ph or substituted Ph; R3 = H, Cl, CN, Et, CH2NH2, etc.) II (R and R1 = H, OH, MeO; X = CN, CONH2, CONHAc) and III (R and R1 = F, OH, AcO; R2 = C5-7 cyclic) most of which were prepared, were screened for antiinflammatory activity by measuring inhibition of prostaglandin synthetase [9055-65-6] in bovine seminal vesicle microsomes. Many are potent inhibitors of the enzyme with several showing activity at low concentration (IC50 .apprx.4 + 10-8 M) which is 2 order of magnitude lower than the active concentration of known nonsteroidal antiinflammatory agents. Structure-activity relations are discussed.
IT **35364-39-7P 66422-13-7P 82925-22-2P**
82925-23-3P 82925-24-4P 82925-25-5P
82925-26-6P 84836-18-0P 84836-19-1P
84836-20-4P 84836-21-5P 84836-22-6P
84836-23-7P 84836-24-8P 84836-25-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and prostaglandin synthetase-inhibiting activity of)
RN 35364-39-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-4-methoxy- (9CI) (CA INDEX NAME)

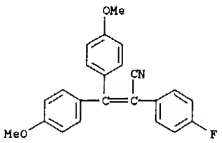
L6 ANSWER 94 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 66422-13-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



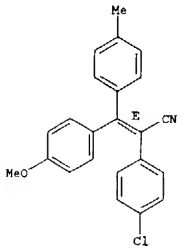
RN 82925-22-2 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-4-fluoro- (9CI) (CA INDEX NAME)



RN 82925-23-3 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

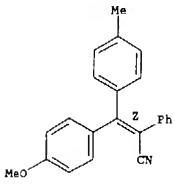
Double bond geometry as shown.

L6 ANSWER 94 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 82925-24-4 CAPLUS
CN Benzeneacetonitrile, α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

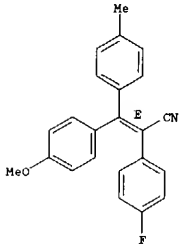
Double bond geometry as shown.



RN 82925-25-5 CAPLUS
CN Benzeneacetonitrile, 4-fluoro-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

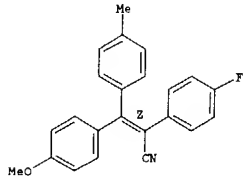
Double bond geometry as shown.

L6 ANSWER 94 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 82925-26-6 CAPLUS
CN Benzeneacetonitrile, 4-fluoro-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

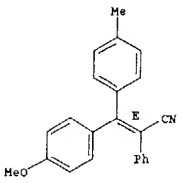
Double bond geometry as shown.



RN 84836-18-0 CAPLUS
CN Benzeneacetonitrile, α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

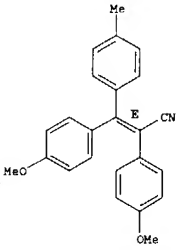
Double bond geometry as shown.

L6 ANSWER 94 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 84836-19-1 CAPLUS
CN Benzeneacetonitrile, 4-methoxy-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



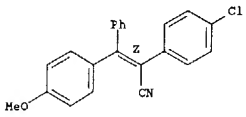
RN 84836-20-4 CAPLUS
CN Benzeneacetonitrile, 4-methoxy-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L6 ANSWER 94 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

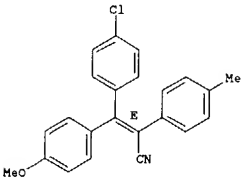
RN 84836-23-7 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[(4-methoxyphenyl)phenylmethylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

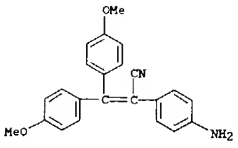


RN 84836-24-8 CAPLUS
CN Benzeneacetonitrile, α-[(4-chlorophenyl)(4-methoxyphenyl)methylene]-4-methyl-, (E)- (9CI) (CA INDEX NAME)

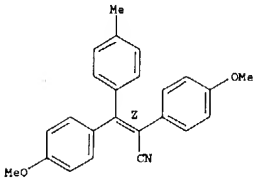
Double bond geometry as shown.



RN 84836-25-9 CAPLUS
CN Benzeneacetonitrile, 4-amino-α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

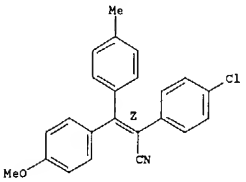


L6 ANSWER 94 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



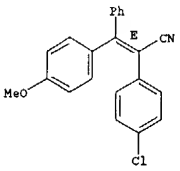
RN 84836-21-5 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



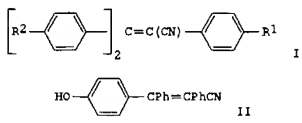
RN 84836-22-6 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[(4-methoxyphenyl)phenylmethylene]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L6 ANSWER 95 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:555928 CAPLUS
DOCUMENT NUMBER: 97:155928
TITLE: Factorial analysis of structure-activity relations of di- and triphenylethylenes in two biochemical tests
AUTHOR(S): Dore, Jean Christophe; Gilbert, Jacques; Crastes de Paulet, Andre; Michel, Francoise; Miquel, Jean Francois
CORPORATE SOURCE: Cent. Etud. Rech. Chim. Org. Appl., Ec. Natl. Super. Chim. Paris, Thiais, 94320, Fr.
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences, Serie 3: Sciences de la Vie (1982), 294(15), 731-4
CODEN: CRSEDA; ISSN: 0249-6313
DOCUMENT TYPE: Journal
LANGUAGE: French
GI



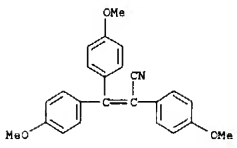
I

II

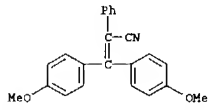
AB The phenylethylenes examined by factorial anal. for inhibitory activity against glutamate dehydrogenase (GDH) [9001-46-1] and prostaglandin synthetase (PGS) [9055-65-6] fell into 1 of 4 classes. 4,4'-Dihydroxy-1,1-diphenylethylenes were markedly active against GDH and only weakly active against PGS. Triphenylacrylonitriles I (R1 = F, Cl, OMe; R2 = Me, OMe) were very active against PGS and weak inhibitors of GDH. Compds. of basic structure II were active against both enzymes. Hydrogenation of the ethylene or substitution of the CN of II with CO2H or CONH2 resulted in inactive compds.

IT **35364-39-7 66422-13-7 82925-21-1 82925-22-2 82925-23-3 82925-24-4 82925-25-5 82925-26-6**
RL: BIOL (Biological study)
(glutamate dehydrogenase and prostaglandin synthetase inhibition by, structure in relation to)

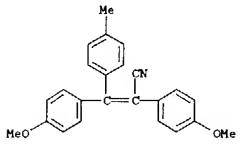
RN 35364-39-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-4-methoxy- (9CI) (CA INDEX NAME)



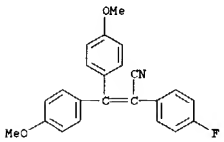
L6 ANSWER 95 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RN 66422-13-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



RN 82925-21-1 CAPLUS
CN Benzeneacetonitrile, 4-methoxy-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]- (9CI) (CA INDEX NAME)



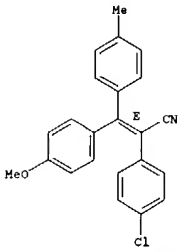
RN 82925-22-2 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-4-fluoro- (9CI) (CA INDEX NAME)



RN 82925-23-3 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

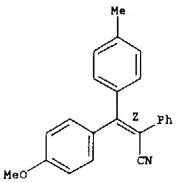
Double bond geometry as shown.

L6 ANSWER 95 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 82925-24-4 CAPLUS
CN Benzeneacetonitrile, α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

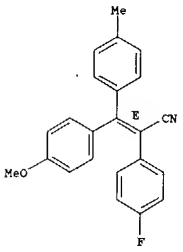
Double bond geometry as shown.



RN 82925-25-5 CAPLUS
CN Benzeneacetonitrile, 4-fluoro-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (E)- (9CI) (CA INDEX NAME)

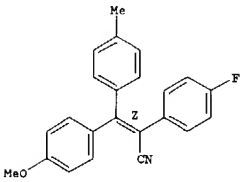
Double bond geometry as shown.

L6 ANSWER 95 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

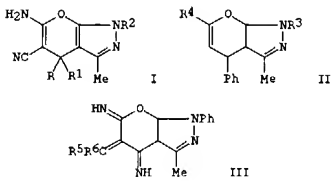


RN 82925-26-6 CAPLUS
CN Benzeneacetonitrile, 4-fluoro-α-[(4-methoxyphenyl)(4-methylphenyl)methylene]-, (Z)- (9CI) (CA INDEX NAME)

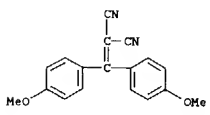
Double bond geometry as shown.



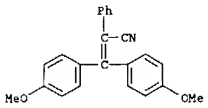
L6 ANSWER 96 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1982:104138 CAPLUS
DOCUMENT NUMBER: 96:104138
TITLE: Activated nitriles in heterocyclic synthesis: a novel synthesis of pyrano[2,3-c]pyrazoles
AUTHOR(S): Abdou, Sadek; Fahmy, Sherif Mahmoud; Sadek, Kamal Usef; Elnagdi, Mohamed Hilmy
CORPORATE SOURCE: Fac. Sci., Minia Univ., Egypt
SOURCE: Heterocycles (1981), 16(12), 2177-80
CODEN: HTCYAM; ISSN: 0385-5414
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 96:104138
GI



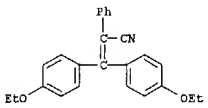
AB Pyranopyrazoles I [R = (un)substituted Ph, R1 = H, (un)substituted Ph, R2 = H, Ph, RR1 = 9-fluorenylidenyl], II (R3 = H, Ph, R4 = OH, Ph), and III (R5 = Ph, p-MeOC6H4, m-O2NC6H4, R6 = H; R5 = R6 = Ph, p-MeOC6H4; R5R6 = 9-fluorenylidenyl) were prepared in 50-94% yields by cyclocondensation reactions of phenylacrylonitriles with 3-methyl- and 3-methyl-1-phenyl-2-pyrazolin-5-ones.
IT **21453-19-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with methyl- and methylphenylpyrazolinones)
RN 21453-19-0 CAPLUS
CN Propanedinitrile, [bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



L6 ANSWER 97 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1981:400969 CAPLUS
DOCUMENT NUMBER: 95:969
TITLE: Relation between radioprotection and estrogenic effect of nonsteroidal estrogens
AUTHOR(S): Xu, Xiu-Rong; Zhou, Jie; Wen, Jia-Sheng; Tao, Zheng-Qin; Kang, Ai-Li; Huang, Jia-Xin; Yang, Hui-Hua; Zhou, Pei-Qin
CORPORATE SOURCE: Shanghai Inst. Mater. Med., Acad. Sin., Shanghai, Peop. Rep. China
SOURCE: Yaoxue Xuebao (1980), 15(11), 648-55
CODEN: YHHPAL; ISSN: 0513-4870
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB Primary results on the radioprotection by and estrogenic activity of nonsteroidal estrogens in mice are presented. Of 58 compds. tested, 46 protected against a LD of γ-irradiation (60Co). EDs varied over a wide range (0.002-5.00 mg/animal). The radioprotective and estrogenic activities were not parallel. Estrogenic activity was determined by the uterus weight method.
IT **66422-13-7 77799-34-9 77799-35-0 77799-36-1**
RL: BIOL (Biological study)
(estrogenic activity and radioprotection by)
RN 66422-13-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

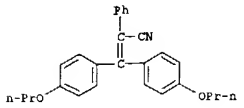


RN 77799-34-9 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-ethoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

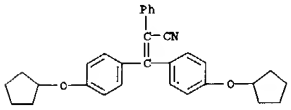


RN 77799-35-0 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-propoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 97 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



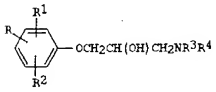
RN 77799-36-1 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-(cyclopentyloxy)phenyl]methylene]- (9CI) (CA INDEX NAME)



L6 ANSWER 98 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1980:495297 CAPLUS
DOCUMENT NUMBER: 93:95297
TITLE: 1-Aryloxy-2-hydroxy-3-aminopropanes
INVENTOR(S): Fritsch, Werner; Stache, Ulrich; Lindner, Ernst
PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
SOURCE: U.S., 16 pp. Cont.-in-part of U.S. Ser. No. 799,676, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

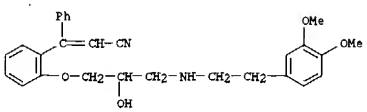
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4191765	A	19800304	US 1978-932504	19780810
DE 2623314	A1	19771208	DE 1976-2623314	19760525
DE 2623314	C2	19840802		
PRIORITY APPLN. INFO.:			US 1977-799676	19770523
			DE 1976-2623314	19770525

GI



I

AB Glycidyl ethers reacted with amines to yield phenoxyisopropanolamines I [R and R1 (same or different) are H, allyl, halo, NO2, alkyl, alkoxy; R2 = CR5:CR6CO2R7 or CR5:CR6CN (R5 = H, alkyl, aryl, aralkyl; R6 = H, alkyl; R7 = H, alkyl, aralkyl); R3 = H and R4 = (un)substituted phenylalkyl or NR3R4 = heterocyclic ring], useful as antiarrhythmics and antihypertensives (no data). 3-(2-Glycidyloxyphenyl)crotononitrile was heated with morpholine in EtOH to give 3-[2-(2-hydroxy-3-morpholinopropoxy)phenyl]crotononitrile.
IT **65655-14-3P 65655-15-4P 65655-16-5P 65655-17-6P 65655-20-1P 65655-21-2P 65715-70-0P 65715-71-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 65655-14-3 CAPLUS
CN 2-Propenenitrile, 3-[2-[3-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-hydroxypropoxy]phenyl]-3-phenyl- (9CI) (CA INDEX NAME)

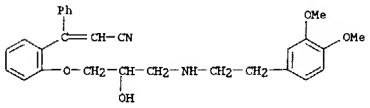


RN 65655-15-4 CAPLUS
CN 2-Propenenitrile, 3-[2-[3-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-

L6 ANSWER 98 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
hydroxypropoxy]phenyl]-3-phenyl-, ethanedioate (2:1) (salt) (9CI) (CA INDEX NAME)

CM 1

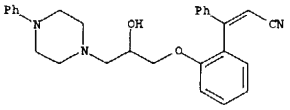
CRN 65655-14-3
CMF C28 H30 N2 O4



CM 2

CRN 144-62-7
CMF C2 H2 O4

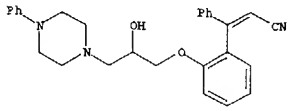
RN 65655-16-5 CAPLUS
CN 2-Propenenitrile, 3-[2-[2-hydroxy-3-(4-phenyl-1-piperazinyl)propoxy]phenyl]-3-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



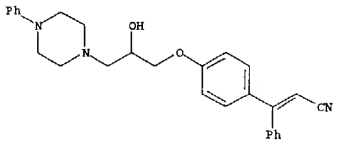
● HCl

RN 65655-17-6 CAPLUS
CN 2-Propenenitrile, 3-[2-[2-hydroxy-3-(4-phenyl-1-piperazinyl)propoxy]phenyl]-3-phenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 98 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

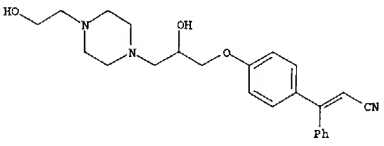


RN 65655-20-1 CAPLUS
CN 2-Propenenitrile, 3-[4-[2-hydroxy-3-(4-phenyl-1-piperazinyl)propoxy]phenyl]-3-phenyl-, dihydrochloride (9CI) (CA INDEX NAME)



●2 HCl

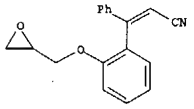
RN 65655-21-2 CAPLUS
CN 2-Propenenitrile, 3-[4-[2-hydroxy-3-[4-(2-hydroxyethyl)-1-piperazinyl]propoxy]phenyl]-3-phenyl-, dihydrochloride (9CI) (CA INDEX NAME)



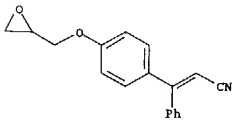
●2 HCl

RN 65715-70-0 CAPLUS

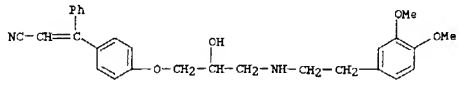
L6 ANSWER 98 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 65591-92-6 CAPLUS
CN 2-Propenenitrile, 3-[4-(oxiranylmethoxy)phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



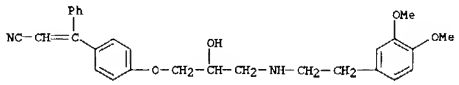
L6 ANSWER 98 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN 2-Propenenitrile, 3-[4-[3-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-hydroxypropoxy]phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



RN 65715-71-1 CAPLUS
CN 2-Propenenitrile, 3-[4-[3-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-hydroxypropoxy]phenyl]-3-phenyl-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 65715-70-0
CMF C28 H30 N2 O4



CM 2

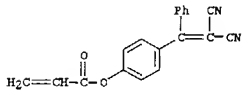
CRN 144-62-7
CMF C2 H2 O4

IT **65591-90-4 65591-92-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring cleavage of, by amines)
RN 65591-90-4 CAPLUS
CN 2-Propenenitrile, 3-[2-(oxiranylmethoxy)phenyl]-3-phenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 99 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1980:408562 CAPLUS
DOCUMENT NUMBER: 93:8562
TITLE: Synthesis of electron acceptor monomers and their copolymers with N-vinylcarbazole
AUTHOR(S): Mulvaney, J. E.; Brand, Richard A.
CORPORATE SOURCE: Dep. Chem., Univ. Arizona, Tucson, AZ, 85721, USA
SOURCE: Macromolecules (1980), 13(2), 244-8
CODEN: MAMOBX; ISSN: 0024-9297
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The strongly electron-accepting monomers o- and p-(2,2-dicyanovinyl)phenyl acrylate, p-(2,2-dicyanovinyl)phenyl methacrylate, p-(2,2-dicyano-1-phenylvinyl)phenyl acrylate and methacrylate, p-(tricyanovinyl)phenyl acrylate, p-CH2:CHC6H4CH:C(CN)2, and p-CH2:CHC6H4C(CN):C(CN)2 were prepared and polymerized with N-vinylcarbazole. The composition, m.p., and UV spectra of the polymers are described.
IT **72892-25-2 72892-27-4**
RL: PRP (Properties)
(composition and spectra of)
RN 72892-25-2 CAPLUS
CN 2-Propenoic acid, 4-(2,2-dicyano-1-phenylethenyl)phenyl ester, polymer with 9-ethenyl-9H-carbazole (9CI) (CA INDEX NAME)

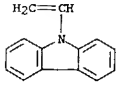
CM 1

CRN 72892-24-1
CMF C19 H12 N2 O2



CM 2

CRN 1484-13-5
CMF C14 H11 N

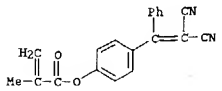


RN 72892-27-4 CAPLUS
CN 2-Propenoic acid, 2-methyl-, 4-(2,2-dicyano-1-phenylethenyl)phenyl ester, polymer with 9-ethenyl-9H-carbazole (9CI) (CA INDEX NAME)

CM 1

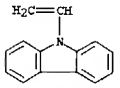
CRN 72892-26-3

L6 ANSWER 99 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CMF C20 H14 N2 O2

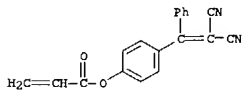


CM 2

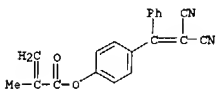
CRN 1484-13-5
CMF C14 H11 N



IT **72892-24-1P 72892-26-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 72892-24-1 CAPLUS
CN 2-Propenoic acid, 4-(2,2-dicyano-1-phenylethenyl)phenyl ester (9CI) (CA INDEX NAME)



RN 72892-26-3 CAPLUS
CN 2-Propenoic acid, 2-methyl-, 4-(2,2-dicyano-1-phenylethenyl)phenyl ester (9CI) (CA INDEX NAME)

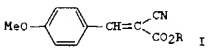


L6 ANSWER 99 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L6 ANSWER 100 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1980:116437 CAPLUS
DOCUMENT NUMBER: 92:116437
TITLE: Light-protective composition containing 4-methoxybenzylidenecyanoacetic acid esters
INVENTOR(S): Preuss, Reinhard; Charlet, Egbert; Finkel, Peter; Rosenkranz, Hans Juergen
PATENT ASSIGNEE(S): Bayer A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 23 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

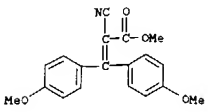
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2816819	A1	19791031	DE 1978-2816819	19780418
US 4284621	A	19810818	US 1979-24742	19790328
EP 5182	A1	19791114	EP 1979-101050	19790406
EP 5182	B1	19810729		
R: BE, CH, DE, FR, GB, IT, NL, SE				
DK 7901563	A	19791019	DK 1979-1563	19790417
AT 7902844	A	19810115	AT 1979-2844	19790417
AT 363603	B	19810825		

PRIORITY APPLN. INFO.: DE 1978-2816819 19780418
GI



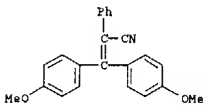
I

AB Light-protective agents against UV of 320-400 nm contained the title compds. I (R = hexyl) [33892-41-0], I (R = octyl) [72955-52-3], I (R = decyl) [41607-83-4], I (R = isononyl) [38722-93-9], or I (R = isodecyl) [72892-43-4]. These compns. may also contain 5-methyl-2-phenylbenzoxazole, 2-phenyl-5-benzimidazolesulfonic acid, or isoamyl 4-methoxycinnamate [71617-10-2], which protect against UV of 285-320 nm. Thus, a sun-protective oil contained I (R = octyl) 2, isoamyl 4-methoxycinnamate 2, peanut oil 46, paraffin oil 50%, and perfume oil.
IT **72955-47-6**
RL: BIOL (Biological study)
(potential sunscreen, UV absorption of)
RN 72955-47-6 CAPLUS
CN 2-Propenoic acid, 2-cyano-3,3-bis(4-methoxyphenyl)-, methyl ester (9CI) (CA INDEX NAME)

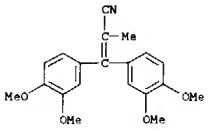


L6 ANSWER 100 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L6 ANSWER 101 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1979:566827 CAPLUS
DOCUMENT NUMBER: 91:166827
TITLE: 3,3-Bis(p-methyloxyphenyl)-2-phenylacrylonitrile
AUTHOR(S): Barrans, Y.; Precigoux, G.; Hospital, M.; Sekera, A.; Miquel, F.
CORPORATE SOURCE: Lab. Cristallogr. Phys. Cryst., Univ. Bordeaux I, Talence, 33405, Fr.
SOURCE: Acta Crystallographica, Section B: Structural Crystallography and Crystal Chemistry (1979), B35(9), 2271-3
CODEN: ACBCAR; ISSN: 0567-7408
DOCUMENT TYPE: Journal
LANGUAGE: French
AB The title compound, C23H19NO2, is monoclinic, space group P21/c, with a 8.595(1), b 9.379(1), c 22.602(2) Å, and β 92.85°; d. (calculated) 1.224 for Z = 4. The structure was solved by direct methods and refined by least-squares to a final R of 0.035. The angles between the 3 aromatic rings are nearly the same as those found in other triphenylethylenes.
IT **66422-13-7**
RL: PRP (Properties)
(structure of)
RN 66422-13-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

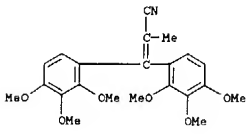


L6 ANSWER 102 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1979:22469 CAPLUS
DOCUMENT NUMBER: 90:22469
TITLE: Reactions of 2-formyl-3-methoxypropionitrile derivatives as electrophilic reagents
AUTHOR(S): Tanaka, Mamoru; Abe, Yasuhiro; Tokuyama, Kanji
CORPORATE SOURCE: Prod. Dep., Shionogi and Co., Ltd., Amagasaki, Japan
SOURCE: Chemical & Pharmaceutical Bulletin (1978), 26(5), 1558-69
CODEN: CPBTAL; ISSN: 0009-2363
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 90:22469
AB The reaction of 2-formyl-3-methoxypropionitrile derivs. (MeO)2CHCR:CH2, MeOCH:CRCH2OMe, (MeO)2CHCHRCH2OMe (R = CN) with benzenes in the presence of an acid catalyst gave cis-MeOCH:CHRCH2R1 (I, R = CN, R1 = Ph, substituted phenyl) and trans-I (R = CO2Me) by electrophilic substitution of the allyl cation. The AlCl3-catalyzed reaction of (EtO)2CHCHRCH2OMe with the benzenes afforded R12CHCHRCH2 by electrophilic substitution of the oxocarbonium ion. In these reactions indan, triphenylpropane, and indene derivs. were obtainable by successive intra- or intermol. substitutions of benzenes at the 2-methoxymethylene groups of I. I were converted into 2-dimethoxymethyl-3-phenylpropionitriles and 2-cyano-1,1-diphenyl-1-propenes, resp., by treatment with NaOMe-MeOH. Some heterocycles such as 3-cyano-2-methoxychroman, 3-cyano-2H-chromene, and 3-cyanoquinoline were similarly derived.
IT **59485-02-8P 68640-42-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 59485-02-8 CAPLUS
CN 2-Propenenitrile, 3,3-bis(3,4-dimethoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)

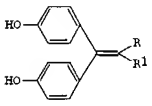


RN 68640-42-6 CAPLUS
CN 2-Propenenitrile, 2-methyl-3,3-bis(2,3,4-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 102 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

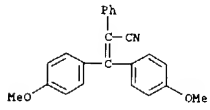


L6 ANSWER 103 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1978:401037 CAPLUS
DOCUMENT NUMBER: 89:1037
TITLE: Synthesis of polyphenylethylenes and their interference with the mouse uterus estrogen receptor
AUTHOR(S): Miquel, Jean Francois; Sekera, Annie; Chaudron, Thierry
CORPORATE SOURCE: CNRS, Thiais, Fr.
SOURCE: Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (1978), 286(4), 151-4
CODEN: CHDCAQ; ISSN: 0567-6541
DOCUMENT TYPE: Journal
LANGUAGE: French
GI



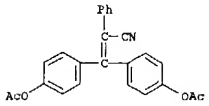
I, R=Cl, R1=CHMe2
II, R=H, R1=Ph

AB Of 16 di-Ph and tri-Ph derivs. of ethylene examined, those showing greatest affinity for the mouse uterus estrogen receptor had free OH substituents on the Ph rings. Acetylation or methylation decreased or eliminated the receptor-binding activity. An addnl. ring in diphenylethylenes on the ethylene C altered their activity. An aliphatic or aliphatic-aromatic side chain on the ethylene C in triphenylethylenes did not appear to alter their activity. The most active of the di- and triphenylethylenes were I [66422-17-1] and II [66422-18-2], resp.
IT **66422-13-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(demethylation of)
RN 66422-13-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



IT **66422-15-9P**
RL: PREP (Preparation)
(preparation of)
RN 66422-15-9 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-(acetyloxy)phenyl]methylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 103 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



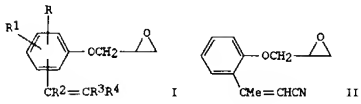
L6 ANSWER 104 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:	1978:89509 CAPLUS
DOCUMENT NUMBER:	88:89509
TITLE:	1-Aryloxy-2,3-epoxypropanes
INVENTOR(S):	Stache, Ulrich; Fritsch, Werner
PATENT ASSIGNEE(S):	Hoechst A.-G., Fed. Rep. Ger.
SOURCE:	Ger. Offen., 23 pp. CODEN: GWXXBX
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2623313	A1	19771215	DE 1976-2623313	19760525
ES 458958	A1	19780216	ES 1977-458958	19770519
NL 7705581	A	19771129	NL 1977-5581	19770520
FI 7701631	A	19771126	FI 1977-1631	19770523
DK 7702270	A	19771126	DK 1977-2270	19770524
SE 7706060	A	19771126	SE 1977-6060	19770524
ZA 7703119	A	19780426	ZA 1977-3119	19770524
AU 7725435	A1	19781130	AU 1977-25435	19770524
AT 7703698	A	19790915	AT 1977-3698	19770524
AT 356125	B	19800410		
HU 20146	O	19810627	HU 1977-HO1986	19770524
HU 177844	P	19811228		
CA 1105041	A1	19810714	CA 1977-279071	19770524
BE 855040	A1	19771125	BE 1977-177908	19770525
FR 2352811	A1	19771223	FR 1977-15887	19770525
JP 53012838	A2	19780204	JP 1977-60003	19770525
PRIORITY APPLN. INFO.:			DE 1976-2623313	19760525

GI



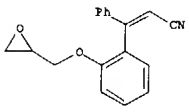
AB Aryloxymethyloxiranes I (R,R1 = H, C1-4 alkyl or alkoxy, allyl, halogen, NO2; R2 = H, C1-5 alkyl, Ph, substituted Ph, phenylalkyl; R3 = H, C1-8 alkyl; R4 = CN, CO2R5; R5 = H, alkyl, aralkyl) were prepared Thus, 2-HOC6H4Ac was treated with epichlorohydrin and the epoxypropoxyacetophenone treated with NCCH2P(O)(OEt)2 to give II.

IT **65591-90-4P 65591-92-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 65591-90-4 CAPLUS

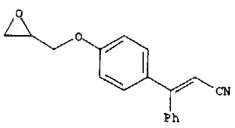
CN 2-Propenenitrile, 3-[2-(oxiranylmethoxy)phenyl]-3-phenyl- (9CI) (CA INDEX NAME)

L6 ANSWER 104 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 65591-92-6 CAPLUS

CN 2-Propenenitrile, 3-[4-(oxiranylmethoxy)phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



L6 ANSWER 105 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

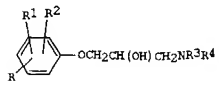
ACCESSION NUMBER:	1978:89351 CAPLUS
DOCUMENT NUMBER:	88:89351
TITLE:	1-Aryloxy-2-hydroxy-3-aminopropanes
INVENTOR(S):	Fritsch, Werner; Stache, Ulrich; Lindner, Ernst
PATENT ASSIGNEE(S):	Hoechst A.-G., Fed. Rep. Ger.
SOURCE:	Ger. Offen., 61 pp. CODEN: GWXXBX
DOCUMENT TYPE:	Patent
LANGUAGE:	German
FAMILY ACC. NUM. COUNT:	2

PATENT INFORMATION:

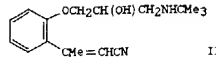
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2623314	A1	19771208	DE 1976-2623314	19760525
DE 2623314	C2	19840802		
ES 458957	A1	19780716	ES 1977-458957	19770519
NL 7705587	A	19771129	NL 1977-5587	19770520
CH 637105	A	19830715	CH 1977-6240	19770520
FI 7701630	A	19771126	FI 1977-1630	19770523
FI 67698	B	19850131		
FI 67698	C	19850510		
SE 7706059	A	19771126	SE 1977-6059	19770524
SE 440903	B	19850826		
SE 440903	C	19851205		
DK 7702271	A	19771126	DK 1977-2271	19770524
ZA 7703120	A	19780426	ZA 1977-3120	19770524
AU 7725434	A1	19781130	AU 1977-25434	19770524
AU 511704	B2	19800904		
AT 7703701	A	19790615	AT 1977-3701	19770524
AT 354421	B	19790110		
CA 1108633	A1	19810908	CA 1977-278974	19770524
HU 21665	O	19820128	HU 1977-HO1987	19770524
HU 179198	B	19820928		
IL 52148	A1	19820730	IL 1977-52148	19770524
BE 855041	A1	19771125	BE 1977-177909	19770525
FR 2353520	A1	19771230	FR 1977-15881	19770525
FR 2353520	B1	19800725		
JP 53012827	A2	19780204	JP 1977-60004	19770525
JP 62014545	B4	19870402		
GB 1577670	A	19801029	GB 1977-22051	19770525
US 4191765	A	19800304	US 1978-932504	19780810
AT 7905197	A	19811215	AT 1979-5197	19790727
AT 367757	B	19820726		
AT 7905198	A	19811215	AT 1979-5198	19790727
AT 367742	B	19820726		
AT 7905199	A	19811215	AT 1979-5199	19790727
AT 367743	B	19820726		
AT 7905200	A	19820215	AT 1979-5200	19790727
AT 368484	B	19821011		
CH 637107	A	19830715	CH 1981-6554	19811013
CH 637108	A	19830715	CH 1981-6555	19811013
CH 637109	A	19830715	CH 1981-6556	19811013
CH 640507	A	19840113	CH 1981-6557	19811013
PRIORITY APPLN. INFO.:			DE 1976-2623314	19760525
			CH 1977-6240	19770520
			US 1977-799676	19770523
			AT 1977-3701	19770524

GI

L6 ANSWER 105 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



I



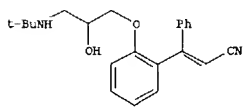
II

AB A series of 67 (±)- or optically active I (R, R1 are H, C1-4 alkyl, allyl, halo, or NO2; R2 is 2-cyano- or -carbalkoxyvinyl or -substituted-vinyl and NR3R4 may be alkylamino or heterocyclylamino) were prepared by reaction of the appropriate amine and epoxide; the compds. were β-sympatholytics and hypotensive agents (no data).

IT **65655-12-1P 65655-13-2P 65655-15-4P**
65655-16-5P 65655-17-6P 65655-18-7P
65655-19-8P 65655-20-1P 65655-21-2P
65715-71-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 65655-12-1 CAPLUS

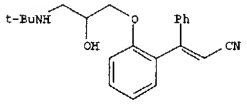
CN 2-Propenenitrile, 3-[2-[3-[(1,1-dimethylethyl)amino]-2-hydroxypropoxy]phenyl]-3-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 65655-13-2 CAPLUS

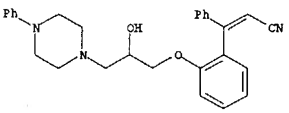
CN 2-Propenenitrile, 3-[2-[3-[(1,1-dimethylethyl)amino]-2-hydroxypropoxy]phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



RN 65655-15-4 CAPLUS

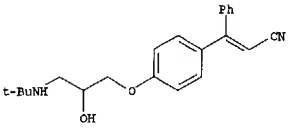
CN 2-Propenenitrile, 3-[2-[3-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-hydroxypropoxy]phenyl]-3-phenyl-, ethanedioate (2:1) (salt) (9CI) (CA

L6 ANSWER 105 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 65655-18-7 CAPLUS

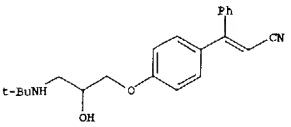
CN 2-Propenenitrile, 3-[4-[3-[(1,1-dimethylethyl)amino]-2-hydroxypropoxy]phenyl]-3-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

RN 65655-19-8 CAPLUS

CN 2-Propenenitrile, 3-[4-[3-[(1,1-dimethylethyl)amino]-2-hydroxypropoxy]phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



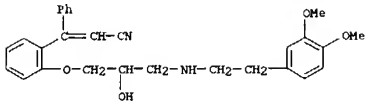
RN 65655-20-1 CAPLUS

CN 2-Propenenitrile, 3-[4-[2-hydroxy-3-(4-phenyl-1-piperazinyl)propoxy]phenyl]-3-phenyl-, dihydrochloride (9CI) (CA INDEX NAME)

L6 ANSWER 105 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CM 1

CRN 65655-14-3
CMF C28 H30 N2 O4

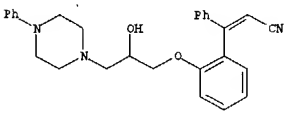


CM 2

CRN 144-62-7
CMF C2 H2 O4

RN 65655-16-5 CAPLUS

CN 2-Propenenitrile, 3-[2-[2-hydroxy-3-(4-phenyl-1-piperazinyl)propoxy]phenyl]-3-phenyl-, monohydrochloride (9CI) (CA INDEX NAME)

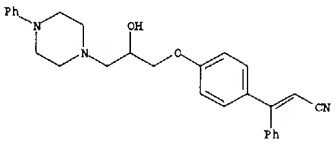


● HCl

RN 65655-17-6 CAPLUS

CN 2-Propenenitrile, 3-[2-[2-hydroxy-3-(4-phenyl-1-piperazinyl)propoxy]phenyl]-3-phenyl- (9CI) (CA INDEX NAME)

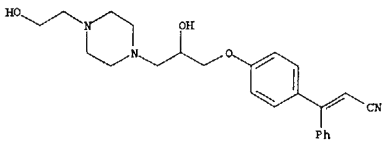
L6 ANSWER 105 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



● 2 HCl

RN 65655-21-2 CAPLUS

CN 2-Propenenitrile, 3-[4-[2-hydroxy-3-[4-(2-hydroxyethyl)-1-piperazinyl]propoxy]phenyl]-3-phenyl-, dihydrochloride (9CI) (CA INDEX NAME)



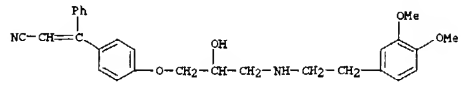
● 2 HCl

RN 65715-71-1 CAPLUS

CN 2-Propenenitrile, 3-[4-[3-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-2-hydroxypropoxy]phenyl]-3-phenyl-, ethanedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 65715-70-0
CMF C28 H30 N2 O4

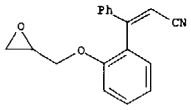


CM 2

L6 ANSWER 105 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CRN 144-62-7
CMF C2 H2 O4

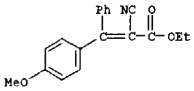
IT **65591-90-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with amines)
RN 65591-90-4 CAPLUS
CN 2-Propenenitrile, 3-[2-(oxiranylmethoxy)phenyl]-3-phenyl- (9CI) (CA INDEX NAME)



L6 ANSWER 106 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:191416 CAPLUS
DOCUMENT NUMBER: 86:191416
TITLE: Discoloration prevention of acrylic laquer compositions
INVENTOR(S): Murakami, Tomohisa; Ueda, Ikuo; Ishino, Teiichi; Nagatomo, Sueo
PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52022029	A2	19770219	JP 1975-97474	19750813
PRIORITY APPLN. INFO.:			JP 1975-97474	19750813

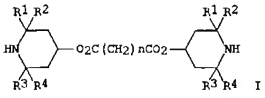
AB Nitrocellulose (I) [9004-70-0]-containing acrylic resin lacquer was mixed with acrylonitrile derivs. and piperidine derivs. to improve the yellowing resistance of the lacquer. Thus, 100 parts of a lacquer comprising I 4.6, an acrylic resin 18.4, di-Bu phthalate 1.3, EtOAc 15.3, BuOAc 11.9, iso-PrOH 11.0, and PhMe 37.5 parts was mixed with 1.4 parts ethylhexyl diphenylmethylenecyanoacetate (II) [6197-30-4] and 0.4 part bis(2,2,6,6-tetramethyl-4-piperidyl) sebacate [52829-07-9], sprayed on a white enamel-coated steel panel and dried to give a coating having superior discoloration resistance to that of a similar coating containing 1.8 parts II alone.
IT **14442-38-7**
RL: USES (Uses)
(discoloration preventers, for coatings)
RN 14442-38-7 CAPLUS
CN 2-Propenoic acid, 2-cyano-3-(4-methoxyphenyl)-3-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 107 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1977:157155 CAPLUS
DOCUMENT NUMBER: 86:157155
TITLE: Polyurethane coating compositions
INVENTOR(S): Murakami, Tomohisa; Ueda, Ikuo; Ishino, Teiichi; Nagatomo, Sueo
PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

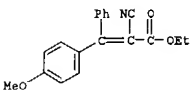
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 52014629	A2	19770203	JP 1975-90183	19750725
PRIORITY APPLN. INFO.:			JP 1975-90183	19750725

GI



I

AB Polyurethane coating compns. having yellowing-resistance were prepared by mixing 5-30% (based on polymers) nitrocellulose and 0.5-10% of a mixture of 1 part acrylonitrile derivative and 0.1-0.5 part piperidine derivative (I, R1-R4 = H or C1-4 alkyl groups, n = 4, 6, 8, 10). Thus, hexamethylene diisocyanate 5.6, Acrydic A-801 (acrylic polyol) 32.6, nitrocellulose 2.3, 2-ethylhexyl diphenylmethylenecyanoacetate [6197-30-4] 0.3, bis(2,2',6,6'-tetramethyl-4-piperidyl) sebacate [52829-07-9] 0.1, MeCOEt 21.5, BuOAc 20.0, cellosolve acetate 6.5, and xylene 11.5 parts were formulated to give a coating composition (dry time to the touch 17 min), which was applied to a primed steel panel to give a 70-μ-thick yellowing-resistant coating (practically no change in 100 h in weatherometer).
IT **14442-38-7**
RL: USES (Uses)
(discoloration preventers, containing piperidine derivs., for nitrocellulose-containing polyurethane coatings)
RN 14442-38-7 CAPLUS
CN 2-Propenoic acid, 2-cyano-3-(4-methoxyphenyl)-3-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 107 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

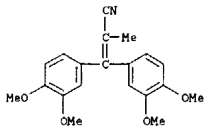
L6 ANSWER 108 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1976:420811 CAPLUS
DOCUMENT NUMBER: 85:20811
TITLE: 3,3-Diphenylpropylamine derivatives
INVENTOR(S): Tokuyama, Kanji; Tanaka, Mamoru
PATENT ASSIGNEE(S): Shionogi and Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 50140431	A2	19751111	JP 1974-44765	19740419
PRIORITY APPLN. INFO.:			JP 1974-44765	19740419

AB Methoxybenzenes (MeO)nC6H6-n (n = 2,3) were treated with MeOCH2CH(CN)CH(OMe)2 (I) in the presence of an acid to give [(MeO)nC6H5-n]2CHCH(CH2OMe)CN (II), which were reduced to [(MeO)nC6H5-n]2CHCH(CH2OMe)CH2NH2 (III) and alkylated to give the N,N-dialkyl derivs. (IV). II were treated with a base to give [(MeO)nC6H5-n]2C:C(CN)Me (V), which were reduced to give [(MeO)nC6H5-n]2C:CMeCH2NH2 (VI). VI were alkylated to give the N,N-dialkyl derivs. (VII). Thus, 1,2-(MeO)2C6H4 was treated with I and AlCl3 3.5 hr at room temperature to give 30% II (n = 2), which (12 g) was reduced with Raney Ni in NH3-MeOH 2 hr at 50-60 atm and 80° to give 10 g III (n = 2), which was refluxed with HCO2H and HCHO 8 hr to give 53.7% IV (n = 2, at positions 3 and 4). II (n = 2) was refluxed in NaOMe-MeOH 2.5 hr to give 87.6% V (n = 2), which (5.1 g) was reduced with Raney Ni to give 4.9 g VI (n = 2), which was refluxed with HCO2H and HCHO to give 61% VII (n = 2, at positions 3 and 4). Similarly prepared were II-VII (n = 3, positions 2, 3, 4).

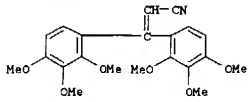
IT **59485-02-8P 59485-03-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)

RN 59485-02-8 CAPLUS
CN 2-Propenenitrile, 3,3-bis(3,4-dimethoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)



RN 59485-03-9 CAPLUS
CN 2-Propenenitrile, 3,3-bis(2,3,4-trimethoxyphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 108 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



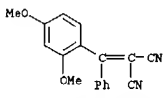
L6 ANSWER 109 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:496943 CAPLUS
DOCUMENT NUMBER: 83:96943
TITLE: Cyclization of ylidenemalononitriles. VIII. Synthesis of coumarins from o-methoxybenzylidenemalonitriles
AUTHOR(S): Campaigne, E.; Mais, Dale E.
CORPORATE SOURCE: Chem. Lab., Indiana Univ., Bloomington, IN, USA
SOURCE: Journal of Heterocyclic Chemistry (1975), 12(2), 267-71
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 83:96943

GI For diagram(s), see printed CA Issue.

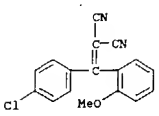
AB The coumarins I (R = H, Cl; R1 = H, 6-,7-,8-MeO) were prepared by direct cyclization of α-cyano-o-methoxycinnamates (II) in H2SO4. Alkoxy groups other than the o-methoxy group involved in lactone formation are not hydrolyzed during the reaction. The 3-cyano group on the resulting coumarin is not hydrated in concentrated H2SO4, but can be converted to the carbamido group in 90% sulfuric acid. In certain cases these conditions do cleave methoxy substituents on the coumarins. The indenones III can be obtained by cyclizing the II with BF3.Et2O.

IT **17212-44-1 56822-04-9 56822-05-0**
56822-06-1 56822-07-2 56822-08-3
56822-09-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(ring closure of)

RN 17212-44-1 CAPLUS
CN Propanedinitrile, [(2,4-dimethoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

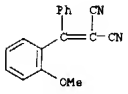


RN 56822-04-9 CAPLUS
CN Propanedinitrile, [(4-chlorophenyl)(2-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

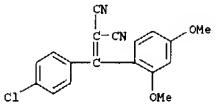


RN 56822-05-0 CAPLUS
CN Propanedinitrile, [(2-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

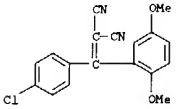
L6 ANSWER 109 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



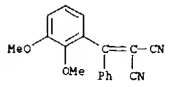
RN 56822-06-1 CAPLUS
CN Propanedinitrile, [(4-chlorophenyl)(2,4-dimethoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



RN 56822-07-2 CAPLUS
CN Propanedinitrile, [(4-chlorophenyl)(2,5-dimethoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

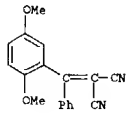


RN 56822-08-3 CAPLUS
CN Propanedinitrile, [(2,3-dimethoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

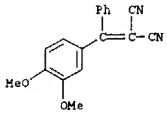


RN 56822-09-4 CAPLUS
CN Propanedinitrile, [(2,5-dimethoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

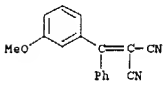
L6 ANSWER 109 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L6 ANSWER 110 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:72613 CAPLUS
DOCUMENT NUMBER: 82:72613
TITLE: New synthesis of ylidenemalononitriles
AUTHOR(S): Campaigne, E.; Mais, Dale; Yokley, E. M.
CORPORATE SOURCE: Dep. Chem., Indiana Univ., Bloomington, IN, USA
SOURCE: Synthetic Communications (1974), 4(6), 379-88
CODEN: SYNCAV; ISSN: 0039-7911
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Nineteen nitriles RR1C:C(CN)2 (I; R,R1 = e.g., Ph substituted Ph, Me3C, 2-benzo[b]thienyl) were prepared by reaction of organometallic compds. with nitriles to give metal ketimates RR1C:NM (M = Li or MgBr), which with 2 equiv CH2(CN)2 gave I. The organometallic compds. were formed by conventional methods. Thus, BuLi in ether at -78° was treated with ether solns. of p-ClC6H4Br, 3,4-(MeO)2C6H3CN, and then CH2(CN)2 and the mixture warmed to room temperature to give 78% I [R = p-ClC6H4, R1 = 3,4-(MeO)2C6H3].
IT **54373-88-5P 54373-90-9P 54373-98-7P**
54373-99-8P 54374-00-4P 54450-83-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 54373-88-5 CAPLUS
CN Propanedinitrile, [(3,4-dimethoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

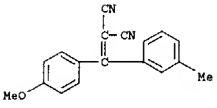


RN 54373-90-9 CAPLUS
CN Propanedinitrile, [(3-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

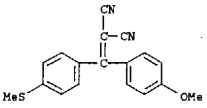


RN 54373-98-7 CAPLUS
CN Propanedinitrile, [(4-methoxyphenyl)(3-methylphenyl)methylene]- (9CI) (CA INDEX NAME)

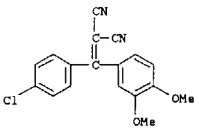
L6 ANSWER 110 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



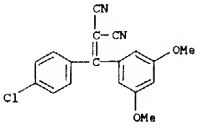
RN 54373-99-8 CAPLUS
CN Propanedinitrile, [(4-methoxyphenyl)[4-(methylthio)phenyl]methylene]- (9CI) (CA INDEX NAME)



RN 54374-00-4 CAPLUS
CN Propanedinitrile, [(4-chlorophenyl)(3,4-dimethoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

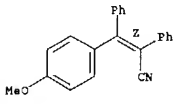


RN 54450-83-8 CAPLUS
CN Propanedinitrile, [(4-chlorophenyl)(3,5-dimethoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

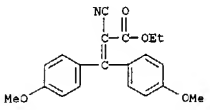


L6 ANSWER 111 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1975:38963 CAPLUS
DOCUMENT NUMBER: 82:38963
TITLE: Triarylhaloethylenes as gonadotropin inhibitors
AUTHOR(S): Palopoli, Frank P.; Feil, Vernon J.; Holtkamp, Dorsey E.; Richardson, Alfred, Jr.
CORPORATE SOURCE: Merrell-Natl. Lab., Div., Richardson-Merrell Inc., Cincinnati, OH, USA
SOURCE: Journal of Medicinal Chemistry (1974), 17(12), 1333-5
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Eight title compds. were prepared by chlorination of the appropriate triarylethylene or etherification of the corresponding phenolic triarylethylene. Of 4 active compds., 1-chloro-1-[p-(β-diethylaminoethoxy)phenyl]-2,2-diphenylethylene-HCl (I-HCl) [53775-02-3] gave 35% lower mean relative ventral prostate weight in rats at 3 mg/kg/day.
IT **53775-13-6**
RL: RCT (Reactant); RACT (Reactant or reagent)
(demethylation of)
RN 53775-13-6 CAPLUS
CN Benzeneacetonitrile, α-[(4-methoxyphenyl)phenylmethylene]-, (Z)- (9CI) (CA INDEX NAME)

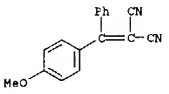
Double bond geometry as shown.



L6 ANSWER 112 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1974:2706 CAPLUS
DOCUMENT NUMBER: 80:2706
TITLE: Chemical shift of protons and dipole moments of a series of dinitriles and ethylenenitrile esters
AUTHOR(S): Rivet-Le Guellec, Paulette; Tonnard, Francois; Meinnel, Jean
CORPORATE SOURCE: Dep. Phys. Crist. Chim. Struct., Univ. Rennes, Rennes, Fr.
SOURCE: Journal de Chimie Physique et de Physico-Chimie Biologique (1973), 70(9), 1268-77
CODEN: JCPBAN; ISSN: 0021-7689
DOCUMENT TYPE: Journal
LANGUAGE: French
AB The proton NMR spectra of some benzalmalononitriles and some Z and E Et α-cyanocinnamic esters have been analyzed. The comparison between exptl. and calculated chemical shifts of vinyl and aromatic protons has given some information about the structure of these compds.: cycle position in reference to the plane of the ethylenic double bond and ester group conformation. These results agreed with those provided by the study of the dipole moments of these compds.
IT **14442-41-2 17212-45-2 21453-19-0 50737-54-7 50737-56-9**
RL: PRP (Properties)
(NMR spectrum of)
RN 14442-41-2 CAPLUS
CN 2-Propenoic acid, 2-cyano-3,3-bis(4-methoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

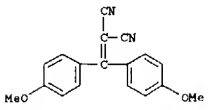


RN 17212-45-2 CAPLUS
CN Propanedinitrile, [(4-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)



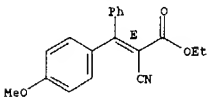
RN 21453-19-0 CAPLUS
CN Propanedinitrile, [bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 112 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



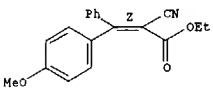
RN 50737-54-7 CAPLUS
CN 2-Propenoic acid, 2-cyano-3-(4-methoxyphenyl)-3-phenyl-, ethyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 50737-56-9 CAPLUS
CN 2-Propenoic acid, 2-cyano-3-(4-methoxyphenyl)-3-phenyl-, ethyl ester, (Z)- (9CI) (CA INDEX NAME)

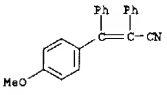
Double bond geometry as shown.



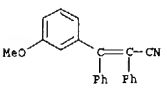
L6 ANSWER 113 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1973:135880 CAPLUS
DOCUMENT NUMBER: 78:135880
TITLE: Aminoalkoxy- or aminomethyltriarylalkenones
INVENTOR(S): Palopoli, Frank P.; Benson, Harvey D.
PATENT ASSIGNEE(S): Richardson-Merrell Inc.
SOURCE: U.S., 5 pp. Division of U.S. 3,634,517 (CA 76:99346w).
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3721712	A	19730320	US 1971-128200	19710325
US 3634517	A	19720111	US 1968-753741	19680819
PRIORITY APPLN. INFO.:			US 1968-753741	19680819

GI For diagram(s), see printed CA Issue.
AB Thirty title compds. [I, R = Me, Bu; R1, R2, R3 = H, Cl, F, Me, MeO, Me2NCH2, OH, Et2N(CH2)2O], having estrogenic or antiestrogenic acitivity at 0.3-250 mg/kg and antiinflammatory activity at 1-20 mg/kg, were prepared Thus, MeLi prepared in situ from MeI and Li, was added to p-MeOC6H4)CPh:CPhCN in Et2O, the solution refluxed 1 hr, hydrolyzed, and converted into the imine HCl salt, which was hydrolyzed to give a mixture of cis-and trans-I (R = Me, R1 = R2 = H, R3 = p-MeO).
IT **35363-69-0 35363-85-0 35364-39-7 35364-41-1 40682-94-8**
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methyl lithium)
RN 35363-69-0 CAPLUS
CN Benzeneacetonitrile, α-[(4-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

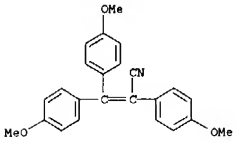


RN 35363-85-0 CAPLUS
CN Benzeneacetonitrile, α-[(3-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

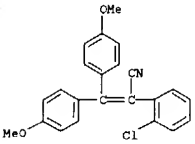


RN 35364-39-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-4-methoxy- (9CI) (CA INDEX NAME)

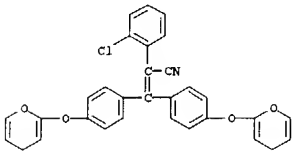
L6 ANSWER 113 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 35364-41-1 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-2-chloro- (9CI) (CA INDEX NAME)



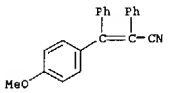
RN 40682-94-8 CAPLUS
CN Benzeneacetonitrile, α-[bis[4-(4H-pyran-2-yloxy)phenyl]methylene]-2-chloro- (9CI) (CA INDEX NAME)



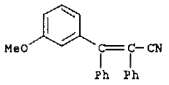
L6 ANSWER 114 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1972:99346 CAPLUS
DOCUMENT NUMBER: 76:99346
TITLE: Triarylalkenones having estrogenic, antiestrogenic, and antiinflammatory activities
INVENTOR(S): Palopoli, Frank P.; Benson, Harvey D.
PATENT ASSIGNEE(S): Richardson-Merrell Inc.
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3634517	A	19720111	US 1968-753741	19680819
US 3721712	A	19730320	US 1971-128200	19710325
PRIORITY APPLN. INFO.:			US 1968-753741	19680819

GI For diagram(s), see printed CA Issue.
AB Thirty pharmacol. active triarylalkenones (I, R1 = alkyl, R2-R5 = H, alkyl, alkoxy, halogen, OH, CF3, or dialkylaminomethyl) were prepared Thus, MeLi from 14.1 g MeI and 1.75 g Li was refluxed 1 hr with 10 g 2,3-diphenyl-3-(p-methoxyphenyl)acrylonitrile in ether to give cis- and trans-I (R1 = Me, R2 = OMe, R3-R5 = H).
IT **35363-69-0 35363-85-0 35364-39-7**
35364-41-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methyllithium)
RN 35363-69-0 CAPLUS
CN Benzeneacetonitrile, α-[(4-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

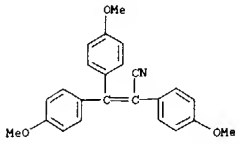


RN 35363-85-0 CAPLUS
CN Benzeneacetonitrile, α-[(3-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

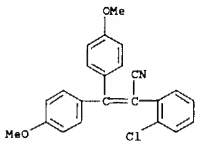


RN 35364-39-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-4-methoxy-

L6 ANSWER 114 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(9CI) (CA INDEX NAME)



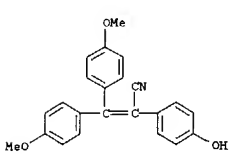
RN 35364-41-1 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-2-chloro- (9CI) (CA INDEX NAME)



L6 ANSWER 115 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1970:100332 CAPLUS
DOCUMENT NUMBER: 72:100332
TITLE: Uterotrophic and gonadotrophic inhibiting 3,3-bis-substituted-(phenyl)-2-(4-hydroxyphenyl)acrylonitriles
INVENTOR(S): Allen, Robert Edward; Ambrus, Laszlo
PATENT ASSIGNEE(S): Cutter Laboratories Inc.
SOURCE: U.S., 3 pp. Continuation-in-part of U.S. 3336255
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3494954	A	19700210	US 1967-647213	19670619
PRIORITY APPLN. INFO.:			US 1967-647213	19670619

GI For diagram(s), see printed CA Issue.
AB A series of the title compds. (I) were prepared by the condensation of an appropriately substituted benzophenone with a (4-alkoxyphenyl)acetonitrile followed by dealkylation of the ether to give a (4-hydroxyphenyl)acetonitrile. Thus, to 110 g benzophenone and 40 g 53% NaH dispersion in mineral oil in 300 ml benzene at reflux was added a solution of 90 g (4-methoxyphenyl)acetonitrile in 200 ml benzene over one hr. The mixture was refluxed 4 addnl. hr and was kept at room temperature 16 hr to give 3,3-diphenyl-2-(4-methoxyphenyl)acrylonitrile-(II), m. 148-9°. II(90 g) and 126 g pyridine-HCl were refluxed 30 min to yield I(R = H)(III), m. 229-30°. III can also be prepared by acid decomposition of 3,3-diphenyl-2-[4-(tetrahydropyran-2-yloxy)phenyl]acrylonitrile, m. 143-4°. Other I prepared were (R and m.p. given): Me, 229-30°; MeO, 217-19°; Cl, 252-4°; Me2N, 240-2°. I have gonadotrophic inhibitory and uterotrophic activity.
IT **16143-94-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 16143-94-5 CAPLUS
CN Acrylonitrile, 2-(p-hydroxyphenyl)-3,3-bis(p-methoxyphenyl)- (8CI) (CA INDEX NAME)



L6 ANSWER 116 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1969:523903 CAPLUS
DOCUMENT NUMBER: 71:123903
TITLE: Urethanes of triarylacrylonitriles
INVENTOR(S): Allen, Robert Edward; Ambrus, Laszlo
PATENT ASSIGNEE(S): Cutter Laboratories Inc.
SOURCE: Brit., 12 pp.
CODEN: BRXXAA
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

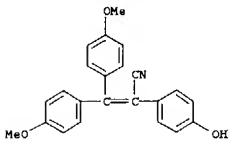
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 1161161		19690813	GB	19670224

AB Title compds., useful for treating animals for fertility and sterility problems stemming from hormonal imbalance, are prepared by the reaction of a hydroxy-containing triphenylacrylonitrile (I) with an isocyanate, cyanic acid, carbamoyl halide, or similar reagent. I may be used as a salt. I is prepared by the demethylation of the corresponding methoxy-substituted triphenylacrylonitrile by pyridine-HCl or by decomposition of the tetrahydro-2H-pyran-2-yl ether of the phenol by aqueous HCl or H2SO4. Thus, to a stirred refluxing suspension of 110 g. Ph2CO and 40 g. NaH (53% in mineral oil) in 300 ml. dry benzene, a solution of 90 g. 4-methoxyphenylacetonitrile in 200 ml. benzene is added over 1 hr., and the mixture refluxed 4 hrs. (to completion of H evolution), held at room temperature 16 hrs., and worked up to give 3,3-diphenyl-2-(4-methoxyphenyl)acrylonitrile, m. 148-9° (alc.). This (90 g.) and 126 g. pyridine-HCl is refluxed 30 min. (no diluent mentioned) and worked up to give 3,3-diphenyl-2-(4-hydroxyphenyl)acrylonitrile, m. 229-30° (alc.). Similarly prepared were the following acrylonitriles (m.p. given): 2-(4-hydroxyphenyl)-3,3-di(4-tolyl)-, 229-30°; 2-(4-hydroxyphenyl)-3,3-bis(4-methoxyphenyl)-, 217-19°; 3,3-bis-(4-chlorophenyl)-2-(4-hydroxyphenyl)-, 252-4°; 2,3-diphenyl-3-(4-hydroxyphenyl)-, 207-8°; 3-(4-hydroxyphenyl)-2-(4-methoxyphenyl)-3-phenyl-, 189-91°; 2-(4-chlorophenyl)-3-(4-hydroxyphenyl)-3-phenyl-(2 geometric isomers, m. 175-7 and 187-9°); 3,3-bis(4-dimethylaminophenyl)-2-(4-hydroxyphenyl)-, 240-2°; 2,3-bis(4-hydroxyphenyl)-3-phenyl-, - (2 geometric isomers, m. 261-2 and 263-4°); 2,3-diphenyl-3-(2-hydroxyphenyl)-, -; and 2-(4-hydroxyphenyl)-3,3-bis(4-trifluoro-methylphenyl)-, -. 3,3-Diphenyl-2-(4-hydroxyphenyl)acrylonitrile (16 g.) in 100 ml. dry benzene containing 10 ml. HCONMe2 and 5 drops pyridine is cooled in an ice bath, 3.4 g. MeNCO in 20 ml. ether added over 20 min. with stirring, and the mixture kept 16 hrs. at room temperature and worked up to give N-methyl-4-(1-cyano-2,2-diphenylvinyl)phenyl carbamate, m. 163-4° (benzene-hexane). The compound has gonadotropic-inhibitory, uterotropic, and myotropic activities. Similarly prepared were the following carbamates (m.p. given): N-methyl 4-[1-cyano-2,2-bis(p-tolyl)vinyl]phenyl, 185-7°; N-methyl 4-[2,2-bis(4-chlorophenyl)-1-cyanovinyl]phenyl, 157-9°; N-methyl 4-[1-cyano-2,2-bis-(4-methoxyphenyl)vinyl]phenyl, 126-8°; N-methyl 4-(2-cyano-1,2-diphenylvinyl)phenyl, yellow, 189-91°; N-phenyl 4-(2-cyano-1,2-diphenylvinyl)phenyl, 178-80°; N-methyl 4-[2-cyano-1,2-diphenylvinyl)phenyl, 178-80°; N-methyl 4-[2-cyano-2-(4-methoxyphenyl)-1-phenylvinyl]phenyl, 175-9°; N-butyl 4-[2-cyano-2-(4-methoxyphenyl)-1-phenylvinyl]phenyl, 164-6°; N-methyl 4-[2-(4-chlorophenyl)-2-cyano-1-phenylvinyl]phenyl, - (geometric isomers, m. 105-7 and

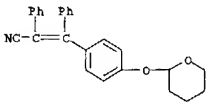
L6 ANSWER 116 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
158-60°); N-propyl 4-(1-cyano-2,2-diphenylvinyl)phenyl, 148-50°; N-phenyl-4 (1-cyano-2,2-diphenylvinyl)phenyl, 170-1°; N,N,dimethyl 4-(1-cyano-2,2-diphenylvinyl)phenyl, 185-6°; N-methyl 4-methyl-4-[1-cyano-2,2-bis(4-dimethylaminophenyl)vinyl]phenyl, 130-2°; N-methyl 2-(2-cyano-1,2-diphenylvinyl)phenyl, -; and N-methyl 4-[1-cyano-2,2-bis(4-trifluoromethylphenyl)vinyl]phenyl, -. Also prepd. was 2,3-bis-[4-(N-methylcarbamoyloxy)phenyl]-3-phenylacrylonitrile (geometric isomers, m. 197-9 and 212-14°).

IT **16143-94-5P 16143-97-8P 16144-00-6P 16144-05-1P 16144-10-8P 16144-11-9P 16144-12-0P 16144-13-1P 16144-14-2P 16144-15-3P 16144-19-7P 16144-20-0P 16255-76-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 16143-94-5 CAPLUS
CN Acrylonitrile, 2-(p-hydroxyphenyl)-3,3-bis(p-methoxyphenyl)- (8CI) (CA INDEX NAME)

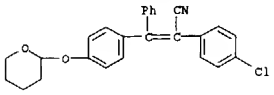


RN 16143-97-8 CAPLUS
CN Acrylonitrile, 2,3-diphenyl-3-[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]- (8CI) (CA INDEX NAME)

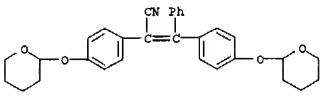


RN 16144-00-6 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[phenyl[4-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]methylene]- (9CI) (CA INDEX NAME)

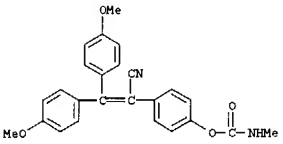
L6 ANSWER 116 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



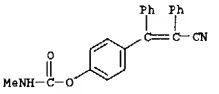
RN 16144-05-1 CAPLUS
CN Acrylonitrile, 3-phenyl-2,3-bis[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]- (8CI) (CA INDEX NAME)



RN 16144-10-8 CAPLUS
CN Carbamic acid, methyl-, ester with 2-(p-hydroxyphenyl)-3,3-bis(p-methoxyphenyl)acrylonitrile (8CI) (CA INDEX NAME)

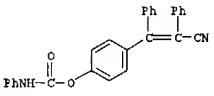


RN 16144-11-9 CAPLUS
CN Carbamic acid, methyl-, ester with 3-(p-hydroxyphenyl)-2,3-diphenylacrylonitrile (8CI) (CA INDEX NAME)

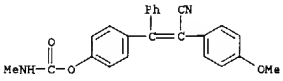


RN 16144-12-0 CAPLUS
CN Acrylonitrile, 3-(p-hydroxyphenyl)-2,3-diphenyl-, carbanilate (ester) (8CI) (CA INDEX NAME)

L6 ANSWER 116 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

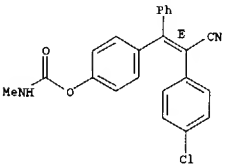


RN 16144-13-1 CAPLUS
CN Carbamic acid, methyl-, ester with 3-(p-hydroxyphenyl)-2-(p-methoxyphenyl)-3-phenylacrylonitrile (8CI) (CA INDEX NAME)



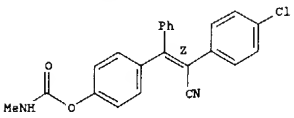
RN 16144-14-2 CAPLUS
CN Carbamic acid, methyl-, ester with 2-(p-chlorophenyl)-3-(p-hydroxyphenyl)-3-phenylacrylonitrile, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 16144-15-3 CAPLUS
CN Carbamic acid, methyl-, ester with 2-(p-chlorophenyl)-3-(p-hydroxyphenyl)-3-phenylacrylonitrile, (Z)- (8CI) (CA INDEX NAME)

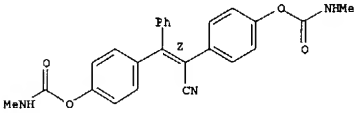
Double bond geometry as shown.



RN 16144-19-7 CAPLUS
CN Carbamic acid, methyl-, diester with 2,3-bis(p-hydroxyphenyl)-3-phenylacrylonitrile, (Z)- (8CI) (CA INDEX NAME)

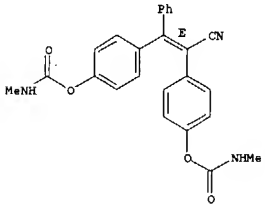
L6 ANSWER 116 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Double bond geometry as shown.

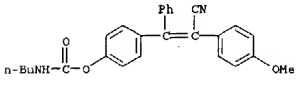


RN 16144-20-0 CAPLUS
CN Carbamic acid, methyl-, diester with 2,3-bis(p-hydroxyphenyl)-3-phenylacrylonitrile, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 16255-76-8 CAPLUS
CN Carbamic acid, butyl-, ester with 3-(p-hydroxyphenyl)-2-(p-methoxyphenyl)-3-phenylacrylonitrile (8CI) (CA INDEX NAME)



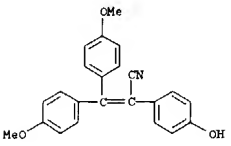
L6 ANSWER 117 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1969:114807 CAPLUS
DOCUMENT NUMBER: 70:114807
TITLE: p-(Cyanovinyl)phenyl carbamates
PATENT ASSIGNEE(S): Cutter Laboratories, Inc.
SOURCE: Fr., 9 pp.
CODEN: FRXXAK
DOCUMENT TYPE: Patent
LANGUAGE: French
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1517437		19680315	FR	19670403

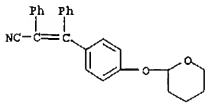
AB p-HOC6H4C(CN):CAr2 (I) and p-HOC6H4C-Ph:CArCN (II) are treated with RNCO compds. and ClCONH2 to give p-(cyanovinyl)phenyl carbamates p-(RNHCO2)C6H4-(CN):CAr2 (III) and p-(RNHCO2)C6H4CPh:CArCN (IV). To a cooled solution of 16 g. p-HOC6H4C(CN):CPh2 in 100 ml. C6H6 containing 10 ml. HCONMe2 and 5 drops pyridine, 3.4 g. MeNCO in 20 ml. Et2O is added in 20 min., and the mixture kept 16 hrs. at room temperature to give 4-(1-cyano-2,2-diphenylvinyl)phenyl N-methylcarbamate, m. 163-4°. Similarly prepared are the following III (R, Ar, and m.p. given): Me, p-tolyl, 185-7°; Me, p-Cl-C6H4, 157-9°; Me, p-MeOC6H4, 126-8°; Pr, Ph, 148-50°; Ph, Ph, 170-1°; H, Ph, -; Me, p-Me2NC6H4, 130-2°; Me, p-F3CC6H4, -. Similarly prepared are IV (R, Ar, and m.p. given): Me, Ph, 189-91°; Ph, Ph, 178-80°; Me, p-MeOC6H4, 175-9°; Bu, p-MeOC6H4, 164-6°; Me, p-ClC6H4, 105-7° and 158-60° (2 geometrical isomers). Also prepared are (m.p. given): p-(Me2NCO2)C6H4C(CN):CPh2, 185-6°; 2,3-bis[4-(N-methylcarbamoyloxy)phenyl]-3-phenylacrylonitrile, 197-9° and 212-14° (geometrical isomers); o-(MeNHCO2)C6H4CPh:C(CN)Ph, -. Also prepared, according to known methods, are the following I (Ar and m.p. given): Ph, 220-30°; p-tolyl, 229-30°; p-MeOC6H4, 217-19°; p-ClC6H4, 252-4°; p-Me2NC6H4, 240-2°; p-F3CC6H4, -; as well as II (Ar and m.p. given): p-MeO-C6H4, 189-91°; p-ClC6H4, 187-9°; p-HOC6H4, 261-2°; o-HO-C6H4C(Ph):C(Ph)CN, p-MeOC6H4C(CN):CPh2, 148-9°; p-MeOC6H4C(CN):C(C6H4Me-p)2, 146-8°; the following 3,3-bis-(Ar-substituted)-2-[4-(tetrahydropyran-2-yloxy)phenyl]acrylonitriles (Ar and m.p. given): Ph, 143-4°; p-Me2NC6H4, 189-91°; the following 2-(Ar-substituted)-3-[4-(tetrahydropyran-2-yloxy)phenyl]-3-phenylacrylonitriles (Ar and m.p. given): Ph, 118-44°; p-ClC6H4, 183-4°; 4-(tetrahydropyran-2-yloxy)phenyl, 189-91°; also p-(tetrahydropyran-2-yloxy)phenylacetonitrile, m. 64-6°; p-(tetrahydropyran-2-yloxy)benzophenone, m. 49-51°

IT **16143-94-5P 16143-97-8P 16144-00-6P 16144-05-1P 16144-10-8P 16144-11-9P 16144-12-0P 16144-13-1P 16144-14-2P 16144-15-3P 16144-19-7P 16144-20-0P 16255-76-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

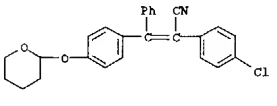
RN 16143-94-5 CAPLUS
CN Acrylonitrile, 2-(p-hydroxyphenyl)-3,3-bis(p-methoxyphenyl)- (8CI) (CA INDEX NAME)



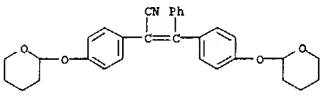
RN 16143-97-8 CAPLUS
CN Acrylonitrile, 2,3-diphenyl-3-[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]- (8CI) (CA INDEX NAME)



RN 16144-00-6 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[phenyl[4-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]methylene]- (9CI) (CA INDEX NAME)

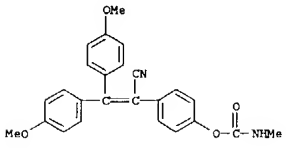


RN 16144-05-1 CAPLUS
CN Acrylonitrile, 3-phenyl-2,3-bis[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]- (8CI) (CA INDEX NAME)

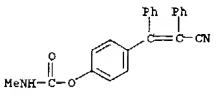


RN 16144-10-8 CAPLUS

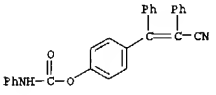
L6 ANSWER 117 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN Carbamic acid, methyl-, ester with 2-(p-hydroxyphenyl)-3,3-bis(p-methoxyphenyl)acrylonitrile (8CI) (CA INDEX NAME)



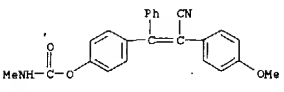
RN 16144-11-9 CAPLUS
CN Carbamic acid, methyl-, ester with 3-(p-hydroxyphenyl)-2,3-diphenylacrylonitrile (8CI) (CA INDEX NAME)



RN 16144-12-0 CAPLUS
CN Acrylonitrile, 3-(p-hydroxyphenyl)-2,3-diphenyl-, carbanilate (ester) (8CI) (CA INDEX NAME)



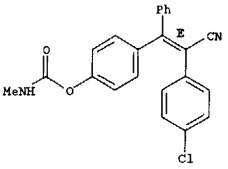
RN 16144-13-1 CAPLUS
CN Carbamic acid, methyl-, ester with 3-(p-hydroxyphenyl)-2-(p-methoxyphenyl)-3-phenylacrylonitrile (8CI) (CA INDEX NAME)



RN 16144-14-2 CAPLUS
CN Carbamic acid, methyl-, ester with 2-(p-chlorophenyl)-3-(p-hydroxyphenyl)-3-phenylacrylonitrile, (E)- (8CI) (CA INDEX NAME)

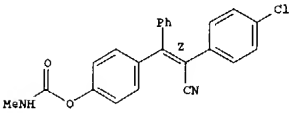
Double bond geometry as shown.

L6 ANSWER 117 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



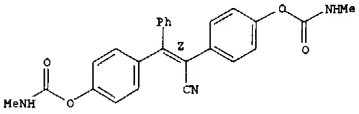
RN 16144-15-3 CAPLUS
CN Carbamic acid, methyl-, ester with 2-(p-chlorophenyl)-3-(p-hydroxyphenyl)-3-phenylacrylonitrile, (Z)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 16144-19-7 CAPLUS
CN Carbamic acid, methyl-, diester with 2,3-bis(p-hydroxyphenyl)-3-phenylacrylonitrile, (Z)- (8CI) (CA INDEX NAME)

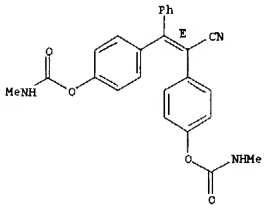
Double bond geometry as shown.



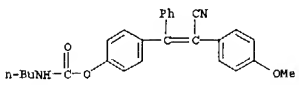
RN 16144-20-0 CAPLUS
CN Carbamic acid, methyl-, diester with 2,3-bis(p-hydroxyphenyl)-3-phenylacrylonitrile, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.

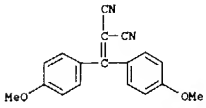
L6 ANSWER 117 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



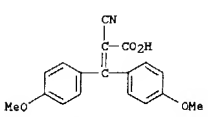
RN 16255-76-8 CAPLUS
CN Carbamic acid, butyl-, ester with 3-(p-hydroxyphenyl)-2-(p-methoxyphenyl)-3-phenylacrylonitrile (8CI) (CA INDEX NAME)



L6 ANSWER 118 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1969:37681 CAPLUS
DOCUMENT NUMBER: 70:37681
TITLE: Carbonyl and thiocarbonyl compounds. XI. Synthesis of halogenated benzodioxoles by the action of tetrahalo-o-benzoquinones on benzophenone hydrazones and their cleavage by nucleophilic reagents
AUTHOR(S): Latif, Nazih; Zeid, I.; Haggag, B.
CORPORATE SOURCE: Nat. Res. Center, Cairo, Egypt
SOURCE: Journal of Heterocyclic Chemistry (1968), 5(6), 831-5
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB p,p'-Dichloro-, p,p'-dimethyl- and p,p'-dimethoxybenzophenone hydrazones react with tetrachloro- and tetrabromo-o-benzoquinone to give directly halogenated benzodioxoles, together with the corresponding tetrahalocatechol. Cleavage of the dioxole ring by nucleophilic reagents depends markedly on the nature of the substituents. The di-MeO analogs proved unusually reactive toward cleavage by dilute mineral acids, LiAlH4, hydrazines and malonitrile, whereas the dichloro analog behaves normally and is not cleaved under the same conditions.
IT **21453-19-0P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 21453-19-0 CAPLUS
CN Propanedinitrile, [bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)



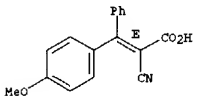
L6 ANSWER 119 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1968:506175 CAPLUS
DOCUMENT NUMBER: 69:106175
TITLE: Structure and physicochemical properties of activated alkenes. II. Synthesis, infrared spectra, and ionization constants of β,β-disubstituted α-cyanoacrylic acids
AUTHOR(S): Le Moal, Henri; Carrie, Robert; Foucaud, Andre; Danion-Bougot, Renee; Gadreau, Claude
CORPORATE SOURCE: Groupe Rech. Physicochim. Struct., Fac. Sci. Rennes, Rennes, Fr.
SOURCE: Bulletin de la Societe Chimique de France (1968), (5), 2156-62
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French
OTHER SOURCE(S): CASREACT 69:106175
GI For diagram(s), see printed CA Issue.
AB trans-α-Cyanocinnamic acid (I), m. 180°, and the following II (R, R1, and m.p. given): p-O2NC6H4, H, 210°; p-ClC6H4, H, 200°; p-tolyl, H, 213°; p-MeOC6H4, H, 231°; m-O2NC6H4, H, 179-80°; o-O2NC6H4, H, 242°; p-O2NC6H4, Me, 212°; p-ClC6H4, Me, 240°; Ph, Me, 176°; p-tolyl, Me, 192°; p-MeOC6H4, Me, 210°; m-O2NC6H4, Me, 180°; o-O2NC6H4, Me, 154° (hydrate); Ph, Ph, 212°; p-O2NC6H4, Ph, 96°; p-ClC6H4, Ph, 172°; p-MeOC6H4, Ph, 160°; p-O2NC6H4, p-O2NC6H4, 254-7°; p-ClC6H4, p-ClC6H4, 108° (hydrate); p-MeOC6H4, p-MeOC6H4, 165°; Ph, PhCH2, 114-15°; PhCH2, PhCH, 77-99° (hydrate); Ph, Et, 132°; Ph, Pr, 107°; Ph, iso-Pr, 117°; 1-C10H7,Me, 165°; 2-C10H7, Me, 210°; III (m. 227°); and IV (m. 201°) are prepared according to 4 known methods. Ir data show that the carbonyl group absorbs at 1714-1682 cm.-1; 3 absorption bands are observed in the 1620-1540 cm.-1 region, of which 2 are attributed to the benzene rings and the 3rd to a vc=c vibration. Ir data for p-XC6H4CHMeCH(CN)CO2H, where X is NO2, Cl, Me, and MeO, are also given. Ionization consts. are determined for
I-IV and compared to those of trans-cinnamic acids PhCR:CHCO2H and Ph2C:CRCO2H. The lack of planarity of II (R1 = aryl group) inhibits conjugation (and resonance) and increases acidity; the pK of II (R = R1 = Ph) is 2.55 as compared to 2.82 for I. The acidity decreases in the order R = p-O2NC6H4 > p-ClC6H4 > Ph > p-MeOC6H4 for II (R1 = H, Me, or Ph).
IT **20168-04-1P 20374-61-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 20168-04-1 CAPLUS
CN 2-Propenoic acid, 2-cyano-3,3-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 20374-61-2 CAPLUS
CN Cinnamic acid, α-cyano-p-methoxy-β-phenyl-, (E)- (8CI) (CA INDEX NAME)

L6 ANSWER 119 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

Double bond geometry as shown.



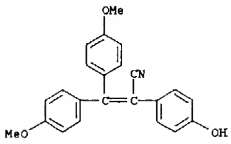
L6 ANSWER 120 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1968:458958 CAPLUS
DOCUMENT NUMBER: 69:58958
TITLE: Urethanes of triarylacrylamides
INVENTOR(S): Allen, Robert E.; Ambrus, Laszlo
PATENT ASSIGNEE(S): Cutter Laboratories, Inc.
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3378579	A	19680416	US 1964-380085	19640702
PRIORITY APPLN. INFO.:			US 1964-380085	19640702

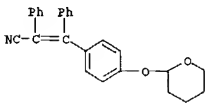
GI For diagram(s), see printed CA Issue.
AB The title compds. (I), in which at least one of the R is a O2CNR2' group, show gonadotrophic inhibitory and uterotrophic, as well as herbicidal and insecticidal activity. They were prepared from the corresponding phenolic triphenylacrylamides and HNCO or an iso-cyanate or a carbamoyl halide. To a refluxing suspension of 110 g. of Ph2CO and 40 g. of NaH (53% in mineral oil) in 300 ml. of C6H6 was added over a period of 1 hr. a solution of 90 g. of 4-MeOC6H4CH2CN in 200 ml. of C6H6. The mixture was refluxed an addnl. 4 hrs., kept at room temperature 16 hrs. to give II (R = R1 = H, R2 = MeO), m. 148-9° (EtOH), which was then demethylated by heating with C5H5N.HCl to II (R = R1 = H, R2 = OH) (III), m. 229-30° (EtOH). III, which has uterotrophic and gonadotrophic inhibitory activities, was also prepared from II (R = R1 = H, R2 = A) (A = tetrahydro-2-pyranyloxy throughout), m. 143-4°. Also prepared were these intermediates: 4-AC6H4CH2CN, m. 64-6° (ether-pentane); 4-AC6H4Bz, m. 49-51°, and II (R, R1, R2, and m.p. given): Me, Me, MeO, 146-8°; Me, Me, OH, 229-30°; MeO, MeO, OH, 217-19°; Cl, Cl, OH, 252-4°; A, H, H, 118-44°; OH, H, H, 207-8°; H, OH, MeO, 189-91°; A, H, Cl, 183-4°; OH, H, Cl, 175-7° and 187-9°; Me2N, Me2N, A, 189-91°; Me2N, Me2N, OH, 240-2°; H, A, A, 189-91°; H, OH, OH, 261-2° and 263-4°. Also prepared was 2,3-diphenyl-3-(2-hydroxyphenyl)acrylonitrile. A mixture of 29.7 g. of III and 120 g. NaOH in 400 g. isoamyl alc. was refluxed 3 hrs. to give I (R = R1 = H, R2 = OH) (IV), m. 284-5° (AcOH). Similarly prepared were the following I (R, R1, and R2 given): Me, Me, OH (m. 254-5°); MeO, MeO, OH; Cl, Cl, OH; H, OH, H; H, OH, MeO; H, OH, Cl; Me2N, Me2N, OH; H, OH, OH. Also described is 2,3-diphenyl-3-(2-hydroxyphenyl)acrylamide. A solution of 2.5 g. MeNCO in 20 ml. of C6H6 was added over a period of 20 min. to a cooled solution of 10 g. of IV, 10 ml. of HCONMe2, and 5 drops of C5H5N in 100 ml. of C6H6, the mixture kept for 16 hrs. at room temperature, and the solvent distilled under reduced pressure to give I (R = R1 = H, R2 = O2CNHMe), m. 234-5° (C6H6).
IT **16143-94-5P 16143-97-8P 16144-00-6P 16144-05-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 16143-94-5 CAPLUS
CN Acrylonitrile, 2-(p-hydroxyphenyl)-3,3-bis(p-methoxyphenyl)- (8CI) (CA

L6 ANSWER 120 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

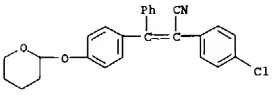
L6 ANSWER 120 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
INDEX NAME)



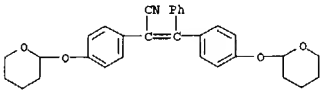
RN 16143-97-8 CAPLUS
CN Acrylonitrile, 2,3-diphenyl-3-[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]- (8CI) (CA INDEX NAME)



RN 16144-00-6 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[phenyl[4-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]methylene]- (9CI) (CA INDEX NAME)



RN 16144-05-1 CAPLUS
CN Acrylonitrile, 3-phenyl-2,3-bis[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]- (8CI) (CA INDEX NAME)



L6 ANSWER 121 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1968:418873 CAPLUS
DOCUMENT NUMBER: 69:18873
TITLE: Ether-linked basic amines of triarylacrylamides
INVENTOR(S): Allen, Robert E.; Ambrus, Laszlo
PATENT ASSIGNEE(S): Cutter Laboratories Inc.
SOURCE: U.S., 7 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

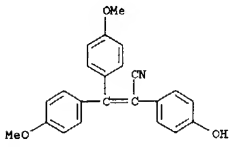
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3361813	A	19680102	US 1964-380086	19640702
PRIORITY APPLN. INFO.:			US 1964-380086	19640702

GI For diagram(s), see printed CA Issue.
AB The title compds. were prepared by reaction of a phenolic hydroxy-containing triarylacrylamide with an aminoalkyl halide. A solution of 90 g. p-MeOC6H4CH2CN in 200 ml. dry C6H6 was added to a stirred refluxing suspension of 110 g. Ph2CO (I) and 40 g. NaH (II) (53% suspension in mineral oil), the mixture refluxed an addnl. 4 hrs., kept at room temperature 16 hrs., excess II decomposed with H2O, and the organic layer separated to give 3,3-diphenyl-2-(r-methoxyphenyl)acrylonitrile (III) (R = R1 = H, R2 = p-OMe) (IV), yellow, m. 148-9°. IV (90 g.) and 126 g. C5H5N.HCl was refluxed 30 min., the mixture cooled, diluted with H2O, and filtered, the crude precipitate dissolved in 1 l. 5% solution NaOH, the resulting solution filtered, and the filtrate acidified with 1 l. 5% solution HCl to give III (R = R1 = H, R2 = p-OH) (V), m. 229-30°. V was also prepared by the acid decomposition of III (R = R1 = H, R2 = tetrahydropyran-2-yloxy), m. .apprx.143-4° [prepared by condensation of I with 4-(tetrahydropyran-2-yloxy)phenylacetonitrile, m. 64-6°]. A mixture of 29.7 g. V and 120 g. NaOH in 400 ml. isoamyl alc. was refluxed 3 hrs., and the mixture cooled to give a precipitate which was dissolved in 500 ml. warm H2O, and repptd. by dilution with excess 10% solution HCl to give 3,3-diphenyl1-2-(4-hydroxyphenyl)acrylamide (VI) (R = R1 = H, R2 = p-OH), m. 284-5°. A mixture of 100 g. p-HOC6H4COPh and 50 g. dihydropyran was dissolved in 500 ml. warm dry C6H6 and 2 ml. concentrated HCl and the mixture refluxed 4 hrs. and kept 16 hrs. at room temperature to give 4-(tetrahydropyran-2-yloxy)benzophenone (VII), m. 49-51° (pentane). To a refluxing suspension of 8 g. II in 200 ml. Et2O a solution of 11.4 g. PhCH2CN in 200 ml. Et2O was added during 2 hrs. and the mixture refluxed an addnl. hr., treated with a solution of 28 g. VII in 100 ml. Et2O, refluxed 2 hrs., and kept 16 hrs. at room temperature to give III (R = R2 = H, R1 = 4-tetrahydropyran-2-yloxy) (VIII), m. 118-44°. A solution of VIII in 100 ml. hot HOAc containing a few drops concentrated H2SO4 diluted with H2O gave III (R = R2 = H, R1 = p-OH), yellow, m. 207-8°. Other III prepared were (R, R1, R2, and m.p. given): p-Me, p-Me, p-OMe, 146-8° (iso-PrOH); p-Me, p-Me, p-OH, 229-30°; p-MeO, p-MeO, p-OH, 217-19°; p-Cl, p-Cl, p-OH, 252-4° (HOAc); p-OH, H, p-MeO, 189-91° (HOAc); p-Q (Q =

L6 ANSWER 121 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
tetrahydropyran-2-yloxy], H, p-Cl, 183-4° (EtOH); p-OH, H, p-Cl, 175-7° and 187-9° (geometric isomers); p-NMe2, p-NMe2, p-Q, 189-91°; p-NMe2, p-NMe2, p-OH, 240-2°; H, p-Q, p-Q, 189-91°; p-OH, H, p-OH, 261-2° and 263-4° (geometric isomers); H, p-OH, H, -; p-CF3, p-CF3, p-MeO, -; p-CF3, p-CF3, p-OH, -. Other VI prepd. were (R, R1, and R2 given): p-Me, p-Me, p-OH, m. 254-5°; p-MeO, p-MeO, p-OH; p-Cl, p-Cl, p-OH; H, p-OH, H; p-OH, H, p-MeO; p-OH, H, p-Cl; p-NMe2, p-NMe2, p-Q, m. 189-91° (HCONMe2-EtOH); p-NMe2, p-NMe2, p-OH; p-OH, H, p-OH; H, p-OH, H; p-CF3, p-CF3, p-OH. Also prepd. were the HCl salts of the following VI (R, R1, and R2 given): H, H, p-O (CH2)2NEt2, m. 104° (iso-PrOH); p-Me, p-Me, p-O (CH2)2NEt2, m. 177-8°; p-Cl, p-Cl, p-O (CH2)2NEt2; p-OH, p-OH, p-O (CH2)2NEt2; H, H, p-O (CH2)2NMe2; H, H, p-O (CH2)3NMe2; p-O (CH2)2NEt2, H, H; p-O (CH2)2NEt2, H, p-MeO; p-O (CH2)2NEt2, H, p-Cl; p-NMe2, p-NMe2, p-O (CH2)2NEt2; p-O (CH2)2NEt2, H, p-O (CH2)2NEt2; o-O (CH2)2NEt2, H, H; p-CF3, p-CF3, p-O (CH2)2NEts. Also prepd. were 3,3-diphenyl-2-[4-(2-piperidinoethoxy)phenyl]acrylamide-HCl and the corresponding 2-(1-pyrrolidinyl)ethoxy analog. A soln. of VI (R = R1 = H, R2 = O(CH2)2NEt2) (0.028 mole) in 300 ml. MeOH treated with 10 ml. 30% H2O2 was kept 20 hrs. at room temp., the solvent removed in vacuo, and the residual oil taken up in 100 ml. EtOAc and acidified to .apprx.pH 2 with alc. HCl soln. to give 2-[4-(2-diethylaminoethoxy)phenyl]-3,3-diphenylacrylamide N-oxide, HCl salt, melted with decompn. The N-oxide base was obtained by working up the product of the H2O2 reaction, and sepg. it without prior acidification. These compds. are characterized by gonadotrophic-inhibitory, and uterotrophic activity, herbicidal, and insecticidal activity. Some compds. exhibit antilipase or lipase inhibitory activity.

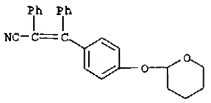
IT **16143-94-5P 16143-97-8P 16144-00-6P**
16144-05-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 16143-94-5 CAPLUS
CN Acrylonitrile, 2-(p-hydroxyphenyl)-3,3-bis(p-methoxyphenyl)- (8CI) (CA INDEX NAME)

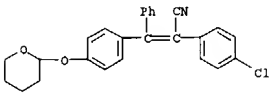


RN 16143-97-8 CAPLUS
CN Acrylonitrile, 2,3-diphenyl-3-[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]- (8CI) (CA INDEX NAME)

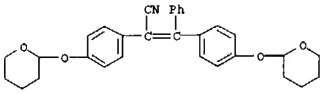
L6 ANSWER 121 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



RN 16144-00-6 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[phenyl[4-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]methylene]- (9CI) (CA INDEX NAME)



RN 16144-05-1 CAPLUS
CN Acrylonitrile, 3-phenyl-2,3-bis[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]- (8CI) (CA INDEX NAME)



L6 ANSWER 122 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

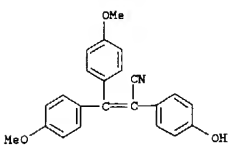
ACCESSION NUMBER: 1968:410284 CAPLUS
DOCUMENT NUMBER: 69:10284
TITLE: Triarylacrylamides
INVENTOR(S): Allen, Robert Edward; Ambrus, Laszlo
PATENT ASSIGNEE(S): Cutter Laboratories Inc.
SOURCE: U.S., 7 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3361790	A	19680102	US 1964-380087	19640702
PRIORITY APPLN. INFO.:			US 1964-380087	19640702

AB To 110 g. Ph2CO and 40 g. 53% NaOH-oil dispersion in 300 ml. dry benzene a solution of 90 g. 4-methoxyphenylacetonitrile in 200 ml. dry benzene is added and the mixture heated to reflux, over 1 hr., refluxed 4 hrs., kept 16 hrs. at room temperature, and worked up to give 3,3-diphenyl-2-(4-methoxyphenyl)acrylonitrile (I), m. 148-9° (EtOH). I (90 g.) reacted with 126 g. pyridine-HCl to give 3,3-diphenyl-2-(4-hydroxyphenyl)acrylonitrile (II), m. 229-30°. A mixture of 29.7 g. II and 120 g. NaOH gave 3,3-diphenyl-2-(4-hydroxyphenyl)acrylamide (III), m. 284-5°. Similarly prepared were: 2-(4-methoxyphenyl)-3,3-di(4-tolyl)acrylonitrile, m. 146-8°; 2-(4-hydroxyphenyl-3,3-di(4-tolyl)acrylonitrile, m. 229-30°; 2-(4-hydroxyphenyl)-3,3-di(4-tolyl)acrylamide, m. 254-5°. A mixture of 15.5 g. III and 2.7 g. of NaOMe in 100 ml. BuOH is brought to reflux, a suspension of 8.1 g. Na chloroacetate in 20 ml. BuOH added, and the mixture refluxed 4 hrs. and worked up to give [4-(1-carbamoyl-2,2-diphenylvinyl)phenoxy]acetic acid, m. 191-2°. Similarly prepared are: Et [4-[1-carbamoyl-2,2-di(4-tolyl)-vinyl]phenoxy]acetate, m. 130-1°; [4-[1-carbamoyl-2,2-di(4-tolyl)vinyl]phenoxy]acetic acid, m. 264-5°. among other compds. The products are characterized by gonadotrophic inhibitory and uterotropic activity and by herbicidal and insecticidal activity.

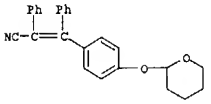
IT **16143-94-5P 16143-97-8P 16144-00-6P**
16144-05-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 16143-94-5 CAPLUS
CN Acrylonitrile, 2-(p-hydroxyphenyl)-3,3-bis(p-methoxyphenyl)- (8CI) (CA INDEX NAME)

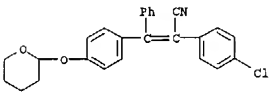


RN 16143-97-8 CAPLUS
CN Acrylonitrile, 2,3-diphenyl-3-[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]-

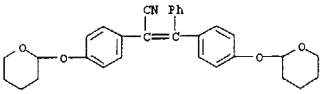
L6 ANSWER 122 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(8CI) (CA INDEX NAME)



RN 16144-00-6 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[phenyl[4-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]methylene]- (9CI) (CA INDEX NAME)



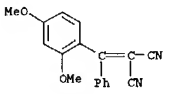
RN 16144-05-1 CAPLUS
CN Acrylonitrile, 3-phenyl-2,3-bis[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]- (8CI) (CA INDEX NAME)



L6 ANSWER 123 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1967:509710 CAPLUS
DOCUMENT NUMBER: 67:109710
TITLE: Ultraviolet stabilizers for nitrocellulose and polyester coatings, lacquers and sheets
INVENTOR(S): Liebig, Horst; Knaul, Joachim
PATENT ASSIGNEE(S): Riedel-de Haen A.-G.
SOURCE: Ger., 3 pp.
CODEN: GWXXAW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

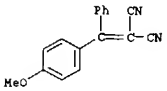
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1242780		19670622	DE	19600715

GI For diagram(s), see printed CA Issue.
AB The title compds. have the advantage of not discoloring in the presence of trace metals such as Fe. In addition they are insol. to alkaline solns., independent of pH, stable against uv and are soluble in solvents such as C6H6, Me2CO, and acetates. Thus, I is prepared by dissolving 24.2 g. 2,4-dimethoxybenzophenone and 11.3 g. cyanoethyl acetate in 100 ml. PhMe. The solution is placed in an apparatus with an H2O separator and 4 g. NH4OAc and 12 ml. AcOH are added. It is then boiled for 5 hrs., neutralized, and the II isolated. After purification by Al2O3 chromatog., II is a viscous, yellow oil, Rf value 0.58 (thinlayer chromatog., silica gel G, CHCl3, developer SbCl5 in CCl4). Other I similarly prepared were (R1, R2, R3, and m.p. given): MeO, MeO, CN, 124-5°; H, MeO, CN, 119-20°; H, H, CN 140-1°; and H, H, CO2Et, -. Transmission values were determined from 320 to 420 μ in 20-μ steps for the various uv stabilizers after 50, 100, and 200 hrs. exposure to a Hg-vapor lamp.
IT **17212-44-1 17212-45-2 17675-63-7**
RL: USES (Uses)
(as ultraviolet light stabilizer for nitrocellulose or polyester coatings or sheets)
RN 17212-44-1 CAPLUS
CN Propanedinitrile, [(2,4-dimethoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

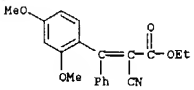


RN 17212-45-2 CAPLUS
CN Propanedinitrile, [(4-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)

L6 ANSWER 123 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



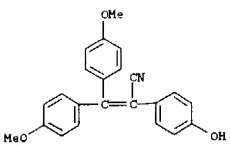
RN 17675-63-7 CAPLUS
CN Acrylic acid, 2-cyano-3-(2,4-dimethoxyphenyl)-3-phenyl-, ethyl ester (8CI) (CA INDEX NAME)



L6 ANSWER 124 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1967:508462 CAPLUS
DOCUMENT NUMBER: 67:108462
TITLE: α-[p-[1(and 2)-Cyanovinyl]phenoxy]alkanoic acids
INVENTOR(S): Allen, Robert Edward; Ambrus, Laszlo
PATENT ASSIGNEE(S): Cutter Laboratories Inc.
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

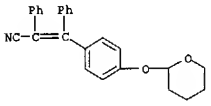
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3336356		19670815	US	19640702

GI For diagram(s), see printed CA Issue.
AB Compds. of the general formulas I and II, which have uterotropic activity and gonadotropic inhibitor activity, are prepared from ArAr1C:CAr2CN (preceding abstract) and X(CH2)nCHRCOY, where X is a halogen, n is 0 or 3, and R is H or an alkyl group. Thus, a mixture of 22 g. p-HOC6H4C(CN):CPh2, 4 g. NaOMe, and 200 ml. BuOH is refluxed, a mixture of 8.6 g. ClCH2CO2Na in 20 ml. BuOH added in 30 min., the mixture refluxed 3 hrs., and the product treated with 10% HCl to give α-[4-(1-cyano - 2,2 - diphenylvinyl)phenoxy]acetic acid, m. 149-50°. Similarly prepared are the following I (Ar, R, and m.p. given): Ph, Et, 109-10°; p-tolyl, H, 154-5°; p-tolyl, Et, 94-5°; p-ClC6H4, Et, 113-15°; p-MeOC6H4, Et, 125-7°; p-Me2NC6H4, Et, -; p-F3CC6H4, H, -; the following II (Ar, R, and m.p. given): Ph, Et, 121-4°; Ph, H, 190-3°; p-MeOC6H4, Et, 112-14°; p-MeOC6H4, H, 202-4°; p-ClC6H4, H, -; p-HO2CCH2OC6H4, H, -; and the following compds. (m.p. given): p-[Ph2C:C(CN)]C6H4OCH2CONH2, 175-6°; p-[(p-ClC6H4)2C:C(CN)] C6H4OCHEtCO2Et, 117-18°; p-[(p-MeOC6H4)2C:C(CN)]C6H4OCHCO2Et, 119-21°; p-[(p-MeOC6H4)2C:C(CN)]C6H4OCH2CONH2, 163-5°; p-[Ph2C:C(CN)]C6H4O(CH2)3CO2H, -; o-(NCC:C)C6H4OCH2CO2H, -.
IT **16143-94-5P 16143-97-8P 16144-00-6P**
16144-05-1P 16149-52-3P 16149-53-4P
16149-54-5P 16149-55-6P 16149-56-7P
16149-57-8P 16149-58-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 16143-94-5 CAPLUS
CN Acrylonitrile, 2-(p-hydroxyphenyl)-3,3-bis(p-methoxyphenyl)- (8CI) (CA INDEX NAME)

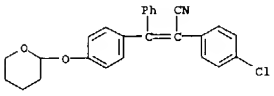


RN 16143-97-8 CAPLUS
CN Acrylonitrile, 2,3-diphenyl-3-[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]-

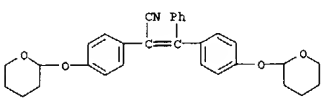
L6 ANSWER 124 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
(8CI) (CA INDEX NAME)



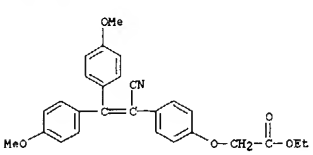
RN 16144-00-6 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[phenyl[4-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]methylene]- (9CI) (CA INDEX NAME)



RN 16144-05-1 CAPLUS
CN Acrylonitrile, 3-phenyl-2,3-bis[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]- (8CI) (CA INDEX NAME)

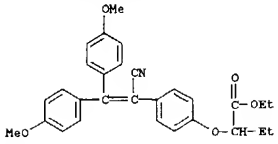


RN 16149-52-3 CAPLUS
CN Acetic acid, [p-[1-cyano-2,2-bis(p-methoxyphenyl)vinyl]phenoxy]-, ethyl ester (8CI) (CA INDEX NAME)

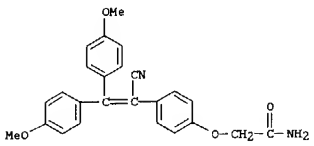


RN 16149-53-4 CAPLUS
CN Butyric acid, 2-[p-[1-cyano-2,2-bis(p-methoxyphenyl)vinyl]phenoxy]-, ethyl ester (8CI) (CA INDEX NAME)

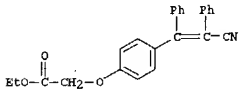
L6 ANSWER 124 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



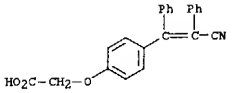
RN 16149-54-5 CAPLUS
CN Acetamide, 2-[p-[1-cyano-2,2-bis(p-methoxyphenyl)vinyl]phenoxy]- (8CI) (CA INDEX NAME)



RN 16149-55-6 CAPLUS
CN Acetic acid, [p-(2-cyano-1,2-diphenylvinyl)phenoxy]-, ethyl ester (8CI) (CA INDEX NAME)

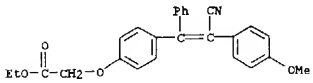


RN 16149-56-7 CAPLUS
CN Acetic acid, [p-(2-cyano-1,2-diphenylvinyl)phenoxy]- (8CI) (CA INDEX NAME)

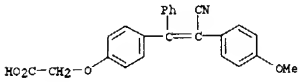


RN 16149-57-8 CAPLUS

L6 ANSWER 124 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
CN Acetic acid, [p-(β-cyano-p-methoxy-α-phenylstyryl)phenoxy]-, ethyl ester (8CI) (CA INDEX NAME)



RN 16149-58-9 CAPLUS
CN Acetic acid, [p-(β-cyano-p-methoxy-α-phenylstyryl)phenoxy]- (8CI) (CA INDEX NAME)



L6 ANSWER 125 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1967:508461 CAPLUS
DOCUMENT NUMBER: 67:108461
TITLE: p-[1(and 2)-Cyanovinyl]phenyl carbamates
INVENTOR(S): Allen, Robert Edward; Ambrus, Laszlo
PATENT ASSIGNEE(S): Cutter Laboratories Inc.
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

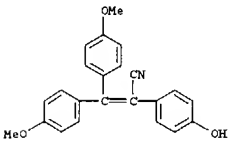
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3336355		19670815	US	19640702

AB ArAr1C:C(CN)C6H4OH-p (I) and NCCAr:CPhC6H4OH-p (II) are prepared and used in the synthesis of compds. III and IV. The cis and trans isomers of 2,3-bis[4-(N-methylcarbamoyloxy)phenyl]-3-phenylacrylonitrile (V) [III (R = H, R1 = Me, Ar = Ph, Ar1 = p-MeNHCO2C6H4)] can be used as uterotropic agents and gonadotropic inhibitors. Thus, a mixture of 110 g. Ph2CO, 0.9 mole NaH (53% dispersion), and 300 ml. C6H6 is refluxed, a solution of 90 g. p-MeOC6H4CH2CN in 200 ml. C6H6 is added in 1 hr., and the mixture refluxed 4 hrs. and kept 16 hrs. at room temperature to give 3,3-diphenyl-2-(4-methoxyphenyl)acrylonitrile, m. 148-9°, which is refluxed with pyridine-HCl to give 3,3-diphenyl-2-(4-hydroxyphenyl)acrylonitrile (VI), m. 229-30°. Similarly prepared are (m.p. given): I (Ar = Ar1 = p-tolyl) (VII) Me ether, 146-8°; VII, 229-30°; I (Ar = Ar1 = p-F3CC6H4), -. Dihydropyran (103 g.) is treated with 160 g. p-HOC6H4CH2CN to give 4-(tetrahydropyran-2-yloxy)phenylacetonitrile (VIII), m. 64-6°. VIII (154 g.) is treated with 174 g. (p-MeOC6H4)2CO in the presence of 70 g. NaNH2 to give I (Ar = Ar1 = p-MeOC6H4), m. 217-19°. Similarly prepared are the following I (Ar = Ar1) (Ar and m.p. given): p-ClC6H4, 252-4°; p-Me2NC6H4, 240-2°. Also prepared is II (Ar = Ar1 = p-Me2NC6H4) tetrahydropyran-2-yl ether, m. 189-91°. Dihydropyran (50 g.) is treated with 100 g. p-HOC6H4COPh (IX) to give IX tetrahydropyran-2-yl ether (X), m. 49-51°. X (28 g.) in 100 ml. Et2O is treated with 11.4 g. PhCH2CN in 200 ml. Et2O in the presence of 8 g. NaNH2 in 200 ml. Et2O to give II (Ar = Ph) tetrahydropyran-2-yl ether (XI), m. 118-44°. Similarly prepared are (m.p. given): II (Ar = p-ClC6H4) (XII) tetrahydropyran-2-yl ether, 183-4°; II (Ar = p-HOC6H4) (XIII) bis(tetrahydropyran-2-yl) ether, 189-91°. XI is treated with HOAc and concentrated H2SO4 to give II (Ar = Ph), m. 207-8°. Similarly prepared are (m.p. given): II (Ar = p-MeOC6H4), 189-91°; XII, 175-7°; XII, 187-9°; XIII, 263-4°; XIII, 261-2°. A solution of 16 g. VI in 100 ml. C6H6 containing .apprx.10 ml. HCONMe2 and .apprx.5 drops pyridine is cooled, 3.4 g. MeNCO in 20 ml. ether added in 20 min., and the mixture kept 16 hrs. at room temperature to give 4-(1-cyano-2,2-diphenylvinyl)phenyl N-methylcarbamate, m. 163-4°. Similarly prepared are the following III (R = H) (R1, Ar, Ar1, and m.p. given): Me, p-tolyl, p-tolyl, 185-7°; Me, p-ClC6H4, p-ClC6H4, 157-9°; Me, p-MeOC6H4, p-MeOC6H4, 126-8°; Pr, Ph, Ph, 148-50°; Ph, Ph, Ph, 170-1°; Me, p-Me2NC6H4, p-Me2NC6H4, 130-2°; Me, p-F3CC6H4, p-F3CC6H4, -; the following IV (R, Ar, and m.p. given): Me, Ph, 189-91°; Ph, Ph, 178-80°; Me, p-MeOC6H4, 175-9°; Bu, p-MeOC6H4, 164-6°; Me, p-ClC6H4, 105-7° and 158-60° (cis and trans isomers). Similarly prepared is a mixture of the cis and trans isomers, m. 197-9° and m. 212-14°, of V. VI is treated with ClCONH2 in the presence of NaOMe to give III (R = R1 = H, Ar = Ar1 = Ph). VI is treated with Me2NCOCl in the presence of NaOMe in HCONMe2 to give III (R = R1 = Me, Ar = Ar1 = Ph). The prepd. III and IV have uterotrotropic and myotrophic activity and can be used as gonadotropic inhibitors.

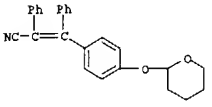
IT **16143-94-5P 16143-97-8P 16144-00-6P**
16144-05-1P 16144-10-8P 16144-11-9P
16144-12-0P 16144-13-1P 16144-14-2P
16144-15-3P 16144-19-7P 16144-20-0P
16255-76-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L6 ANSWER 125 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

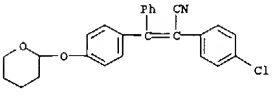
RN 16143-94-5 CAPLUS
CN Acrylonitrile, 2-(p-hydroxyphenyl)-3,3-bis(p-methoxyphenyl)- (8CI) (CA INDEX NAME)



RN 16143-97-8 CAPLUS
CN Acrylonitrile, 2,3-diphenyl-3-[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]- (8CI) (CA INDEX NAME)

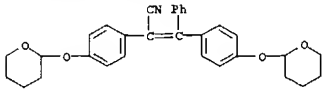


RN 16144-00-6 CAPLUS
CN Benzeneacetonitrile, 4-chloro-α-[phenyl[4-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]methylene]- (9CI) (CA INDEX NAME)

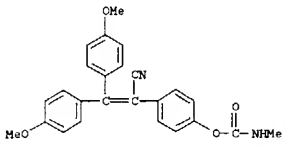


RN 16144-05-1 CAPLUS
CN Acrylonitrile, 3-phenyl-2,3-bis[p-[(tetrahydro-2H-pyran-2-yl)oxy]phenyl]- (8CI) (CA INDEX NAME)

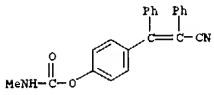
L6 ANSWER 125 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



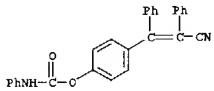
RN 16144-10-8 CAPLUS
CN Carbamic acid, methyl-, ester with 2-(p-hydroxyphenyl)-3,3-bis(p-methoxyphenyl)acrylonitrile (8CI) (CA INDEX NAME)



RN 16144-11-9 CAPLUS
CN Carbamic acid, methyl-, ester with 3-(p-hydroxyphenyl)-2,3-diphenylacrylonitrile (8CI) (CA INDEX NAME)

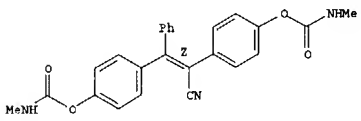


RN 16144-12-0 CAPLUS
CN Acrylonitrile, 3-(p-hydroxyphenyl)-2,3-diphenyl-, carbanilate (ester) (8CI) (CA INDEX NAME)



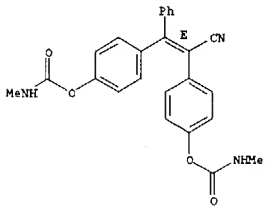
RN 16144-13-1 CAPLUS
CN Carbamic acid, methyl-, ester with 3-(p-hydroxyphenyl)-2-(p-methoxyphenyl)-3-phenylacrylonitrile (8CI) (CA INDEX NAME)

L6 ANSWER 125 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

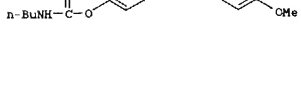


RN 16144-20-0 CAPLUS
CN Carbamic acid, methyl-, diester with 2,3-bis(p-hydroxyphenyl)-3-phenylacrylonitrile, (E)- (8CI) (CA INDEX NAME)

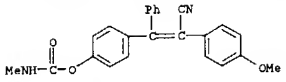
Double bond geometry as shown.



RN 16255-76-8 CAPLUS
CN Carbamic acid, butyl-, ester with 3-(p-hydroxyphenyl)-2-(p-methoxyphenyl)-3-phenylacrylonitrile (8CI) (CA INDEX NAME)

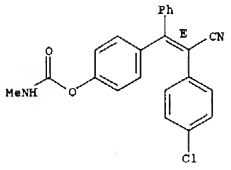


L6 ANSWER 125 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



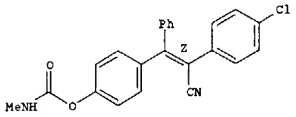
RN 16144-14-2 CAPLUS
CN Carbamic acid, methyl-, ester with 2-(p-chlorophenyl)-3-(p-hydroxyphenyl)-3-phenylacrylonitrile, (E)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 16144-15-3 CAPLUS
CN Carbamic acid, methyl-, ester with 2-(p-chlorophenyl)-3-(p-hydroxyphenyl)-3-phenylacrylonitrile, (Z)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.



RN 16144-19-7 CAPLUS
CN Carbamic acid, methyl-, diester with 2,3-bis(p-hydroxyphenyl)-3-phenylacrylonitrile, (Z)- (8CI) (CA INDEX NAME)

Double bond geometry as shown.

L6 ANSWER 126 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1967:422492 CAPLUS
DOCUMENT NUMBER: 67:22492
TITLE: Ultraviolet stabilizers for polymers
PATENT ASSIGNEE(S): Geigy, J. R., A.-G.
SOURCE: Neth. Appl., 40 pp.
CODEN: NAXXAN
DOCUMENT TYPE: Patent
LANGUAGE: Dutch
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

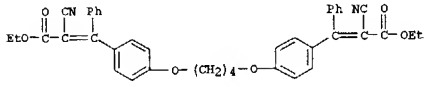
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NL 6610370		19670124		
CH 442218			CH	
DE 1568693			DE	
FR 1487593			FR	
GB 1115596			GB	
US 3546270		19700000	US	
US 3706700		19720000	US	
US 3824273		19740000	US	
PRIORITY APPLN. INFO.:			CH	19650723

AB Bis(methylenemalonic acids) have very little or no color, good stability to light, low sensitivity to alkali or heavy metals, high light absorption and excellent resistance to sublimation, and are used in stabilizing light-sensitive organic material and in the preparation of light filters. From 0.01 to 30% by weight of the uv-absorbing compds. are taken up in light-sensitive polymeric carriers for light filters, depending on the thickness required; e.g. for thin layers of varnish 1-20% by weight and 0.01-1% by weight in thick layers such as polymethacrylate sheets. As carriers, organic thermoplastic and thermosetting polymers can be used, both in synthetic or natural form, or their derivs. Other polymers that are suitable as carriers include homo- and copolymers of vinyl and vinylidene monomers, of epoxy compds., or of lactams and lactones. Suitable condensation polymers are polyesters and polyamides. Suitable natural polymers are largely polysaccharides, rubber, or proteins. Suitable synthetic polymers include reaction products of poly(vinyl alcs.), e.g. poly(vinyl butyral), or saponification products of poly(vinyl esters). Cellulose esters of acetic, propionic, and benzoic acids are also used, as well as synthetic light-sensitive waxes, fats, and oils, or complex systems, such as photographic material and emulsions. At least 1 of the uv-absorbing compds. and other additives are worked into the molten polymer before or during forming, or are dissolved in the monomers before polymerization, or the polymer and addns. are dissolved in a solvent, which is then evaporated The compds. can also be deposited from a bath of an aqueous dispersion on thin carrier material, e.g. films. Thermoplastic synthetic resins are preferred which can be formed at high temperature into articles with a large surface, e.g. polyethylene and isotactic polymers that can be derived from C3-6 alkenes. Antioxidants and their synergists can be applied simultaneously with the light-protecting substances, aniline and naphthalene derivs. being effective. To increase their effectiveness, further synergists can be added, especially high-mol.-weight fatty alc. esters of thiodipropionic acid. To stabilize the color of the artificial resins against heat, phosphites, e.g. Ph3PO3, are added besides the above compds. For example, a solution of 15 g. cellulose acetate with .apprx.2.5 acetoxy groups per glucose unit, together with 0.3 g. of a protective additive,

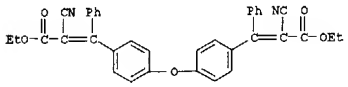
L6 ANSWER 126 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
2.0 g. di-Bu phthalate, and 82.7 g. Me2CO was spread out to form a film on a glass plate. The film formed on evapn. of the Me2CO, was dried at room temp., and then at 60°. Samples of the 0.04-mm.-thick films were exposed to light in a Fade-Ometer and tested from time to time for their content of protective agent and for brittleness. 1,4-Bis[4-(2,2-dicarbethoxyethenyl)phenoxy] butane gave suitable protection, whereas 1,4-bis[4(2-cyano-2-carbethoxyethenyl)phenoxy]butane did not. The former compd. was prepd. by heating for 14 hrs. 19.8 g. 1,4-bis(p-formylphenoxy)butane, 32.0 g. malonic acid di-Et ester, 0.5 g. BzOH, 2 g. piperidine, and 100 ml. C6H6 at its b.p. with a H2O separator. About 3 ml. H2O were sepd. The cooled soln. was filtered and the filtrate concd. by evapn. The honeylike residue crystd. on friction, and was recrystd. from MeOH and ligroine, m.p. 102-3°.

IT **16834-73-4P 16834-76-7P**
RL: PREP (Preparation)
(manufacture of uv-absorbing)

RN 16834-73-4 CAPLUS
CN Acrylic acid, 3,3'-[tetramethylenebis(oxy-p-phenylene)]bis[2-cyano-3-phenyl-, diethyl ester (8CI) (CA INDEX NAME)



RN 16834-76-7 CAPLUS
CN Acrylic acid, 3,3'-(oxydi-p-phenylene)bis[2-cyano-3-phenyl-, diethyl ester (8CI) (CA INDEX NAME)



L6 ANSWER 127 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L6 ANSWER 127 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

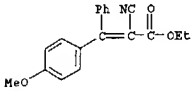
ACCESSION NUMBER: 1967:11443 CAPLUS
DOCUMENT NUMBER: 66:11443
TITLE: Ultraviolet stabilizers for polymer films, fibers, and coatings
INVENTOR(S): Strobel, Albert F.; Catino, Sigmund C.
PATENT ASSIGNEE(S): General Aniline and Film Corp.
SOURCE: Ger., 6 pp.
CODEN: GWXXAW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1222926	C2	19760715	DE 1961-G31781	19610308
PRIORITY APPLN. INFO.:			US 1960-13706	19600309

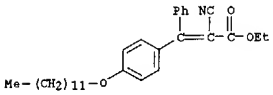
AB Organic-polymer films, fibers, and coatings were protected against uv radiation by addition of 0.1-10% of an α-cyano-β,β-diarylacrylic ester or amide (I). Thus, a mixture of 28.25 g. Et cyanoacetate, 62.75 g. 4,4'-dichlorobenzophenone, 3.85 g. NH4OAc, 12 g. HOAc, and 75 ml. C6H6 was refluxed for 12 hrs. to recover 16 g. ethyl α-cyano-β,β-(4-chlorophenyl)acrylate b2.5 185-200°, m. 81° (2:1 H2O-EtOH). Other substituted (except nitro- or amino-) benzophenones were similarly used to prepare I that were effective uv absorbers, but essentially transparent to visible radiation.

IT **14442-38-7 15646-52-3**
RL: USES (Uses)
(as ultraviolet stabilizer for polymer coatings, fibers and films)

RN 14442-38-7 CAPLUS
CN 2-Propenoic acid, 2-cyano-3-(4-methoxyphenyl)-3-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 15646-52-3 CAPLUS
CN Cinnamic acid, α-cyano-p-(dodecyloxy)-β-phenyl-, ethyl ester (8CI) (CA INDEX NAME)



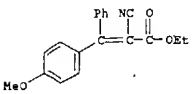
L6 ANSWER 128 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1966:472688 CAPLUS
DOCUMENT NUMBER: 65:72688
ORIGINAL REFERENCE NO.: 65:13497c-f
TITLE: Structure and physicochemical properties of compounds with active ethylenic bonds. I. Synthesis and structure of β,βdisubstituted α-cyanoacrylic esters
AUTHOR(S): Moal, H. Le; Carrie, R.; Foucaud, A.; Bargain, M.; Sevellec, C.
CORPORATE SOURCE: Fac. Sci., Rennes
SOURCE: Bulletin de la Societe Chimique de France (1966), (3), 1033-40
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: French

AB cf. Cope, et al., CA 36, 1011.8 Compds. of the type RR'C:C(CN)CO2Et (I) were synthesized by Cope condensation, where R = p-XC6H4 (X = NO2 or Cl) or 2-naphthyl and R' = Me; R p-XC6H4 (X = MeO, Cl, or NO2) and R' = Ph; R = p-XC6H4 (X = H, Me, or MeO) or 1-naphthyl and R' = Me; and R = Ph and R' = Et, iso-Pr, or PhCH2. When R = Ph and R' = PhCH2, uv spectrum shows that the geometric isomers of I are formed rather than isomers of Ph(PhCH2)C:C(CN)CO2Et and PhHC:C[CH(CN)CO2Et]Ph. The compound is called trans when the substituted or unsubstituted Ph or naphthyl radical is in the trans position relative to the ester function. I gives a more intense band of conjugation and at longer wavelengths for maximum absorption in the uv spectrum. In the ir spectrum, the νc:o frequency is weaker in the case of the trans isomer and stronger in the case of the cis. The absorption bands νc:o of I in CCl4 solution are intense, narrow, and easily recognizable
to within 2 cm.-1 Generally, the pure compds. give a single band and the absorption maximum of the two stereoisomers are generally situated at two different frequencies. The oils, by contrast, manifest two bands (or a band and a marked shoulder). One band has the same frequency as that of the pure solid isomer (when it can be isolated). The other band corresponds to the isomer not isolated from the mixture Gas-phase chromatography using diethylene glycol succinate at 160° with a column pressure drop of 1 kg./cm.2 and a flow rate of 10 ml./sec. gives the best conditions for separation

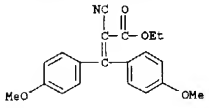
IT **14442-38-7**, Cinnamic acid, α-cyano-p-methoxy-β-phenyl-, ethyl ester **14442-41-2**, Acrylic acid, 2-cyano-3,3-bis(p-methoxyphenyl)-, ethyl ester
(preparation of)

RN 14442-38-7 CAPLUS
CN 2-Propenoic acid, 2-cyano-3-(4-methoxyphenyl)-3-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 14442-41-2 CAPLUS
CN 2-Propenoic acid, 2-cyano-3,3-bis(4-methoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

L6 ANSWER 128 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

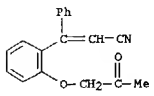


L6 ANSWER 129 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1964:23341 CAPLUS
DOCUMENT NUMBER: 60:23341
ORIGINAL REFERENCE NO.: 60:4121g-h,4122a-e
TITLE: Syntheses with β-arylhydracrylonitriles
AUTHOR(S): Henecka, H.; Lorenz, R.
CORPORATE SOURCE: Farbenfabriken Bayer A.-G., Wuppertal-Elberfeld, Germany
SOURCE: Med. Chem., Abhandl. Med. Chem. Forschungsstaetten Farbenfabriken Bayer A.-G. (1963), 7, 197-214
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB o-Hydroxybenzophenone (247 g.) (from Ph benzoate treated in melted AlCl3-NaCl at 200-20°, in 60-5% yield) in 1400 ml. MeOH containing 70.6 g. NaOMe was treated at -10° dropwise with 175 g. ClCH2OMe to yield 254 g. 2-BzC6H4OCH2OMe (I), b0.3 150°. I (113.3 g.) in 150 ml. Et2O added to a suspension of 25.8 g. NaNH2 in 500 ml. Et2O, 32 g. MeCN added, and the mixture stirred overnight gave 105.4 g. 2-MeOCH2OC6H4CPh(OH)CH2CN (II), m. 120-1.5° (dilute MeOH). II (100 g.) and 20 g. (NH2)2SO2 in 1500 ml. glacial AcOH was heated with 40 ml. 20% H2SO4, and then kept 15 hrs. to give 52 g. 2-HOC6H4CPh:CHCN (III), m. 155-7° (50% AcOH). III (81.7 g.) and 59.3 g. BrCH2Ac in Me2CO was added to a stirred and cooled mixture of powdered K2CO3 and Me2CO, and the mixture stirred overnight to give 101.5 g. 2-AcCH2OC6H4CPh:CHCN (IV), m. 83-4° (dilute MeOH). A 20% solution (3 ml.) of KOH in MeOH was added to 179.6 g. IV in 360 ml. piperidine (exothermic), and the mixture kept 15 hrs. to give 151.7 g. oil. b0.4 176-8°. The oil (228.8 g.) in 500 ml. MeOH gave 80.4 g. crystalline V, m. 115-16°, and the concentrated mother liquor yielded 100.8 g. of the its epimer, m. 66-8°. V (140.8 g. mixture of epimers) in MeOH hydrogenated with Raney Ni at 100°/75-50 atmospheric for 3 hrs. gave 85.7 g. Va (R = H) (VI), b. 150-5° (N-nitroso derivative m. 160-2°). VI (153.7 g.) in 140 ml. MeOH with 454 g. HCO2H and 65 g. 30% formalin gave 51.6 g. α-isomer of Va (R = Me) (α-VII), m. 157°. From the mother liquor were obtained, after high-vacuum distillation, purification via the hydrochlorides, and fractional crystallization, an addnl. 3.7 g. α-VII; 18.2 g. β-VII, m. 107-8°; 4.4 g. γ-VII, m. 140-2°; and 2.2 g. δ-VII (?), m.120-2°. β-Phenyl-β(o-chlorophenyl)hydracrylonitrile(500g.) (prepared from MeCN and o-chlorobenzophenone) in 3 l. MeOH was hydrogenated with Raney Co until 2 moles H were absorbed to give 480 g. 1-phenyl-1-o-chlorophenyl-3-aminopropan-1-ol (VIII), m. 117-19° (aqueous MeOH). N-Methylation of VIII with HCHO-HCO2H yielded dl-1-phenyl-1-(o-chlorophenyl)-3-dimethylaminopropan-1-ol (dl-IX), m. 120-1° (dilute MeOH). β,β-Diphenylhydracrylonitrile (X) (22.3 g.) in 400 ml. EtOH and 85 g. piperidine was hydrogenated over Raney Ni to saturation, and the crude product treated with 11.2 g. Ac2O in 75 ml. C5H5N to give 20 g. crude N-Ac derivative of 1,1-diphenyl-3-aminopropan-1-ol, m. 181-2° (MeOH). The aqueous filtrate was alkalized with NaOH and yielded 3.2 g. N-(γ,γ-diphenyl-γ-hydroxypropyl)piperidine (XI), m. 117-18° (MeOH). XI (17.5 g.) was also obtained by Raney-Ni hydrogenation at 80-90°/80-50 atmospheric of 85 g. piperidine, 60 g. glacial AcOH, and 22.3 g. X in 400 ml. EtOH. The optical isomers of dl-IX were prepared by fractional crystallization of the d-tartrates. d-IX m. 115-16.5°, [α]D 22.25° (CHCl3); HCl salt m. 172-5°, [α]D 8.97°; l-IX m. 115-16°, [α]D -32.2° (CHCl3); HCl salt m. 173-6°, [α]D -12.6° dl-IX showed the same antitussive activity as the optical antipodes.

L6 ANSWER 129 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

IT **93728-92-8**, Cinnamonitrile, o-(acetonyloxy)-β-phenyl- (preparation of)
RN 93728-92-8 CAPLUS
CN Cinnamonitrile, o-(acetonyloxy)-β-phenyl- (7CI) (CA INDEX NAME)



L6 ANSWER 130 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1964:3002 CAPLUS
DOCUMENT NUMBER: 60:3002
ORIGINAL REFERENCE NO.: 60:471h,472a-h
TITLE: Alkylidene formation with imines and active methylene groups. II. Alkylidene derivatives of cyanoacetic acid
AUTHOR(S): Charles, George
CORPORATE SOURCE: Fac. Sci., Poitiers
SOURCE: Bulletin de la Societe Chimique de France (1963), (8-9), 66-72
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB A series of alkylidene derivs. of NCCH2CO2H (I) was prepared from the corresponding ketimines. From α-aryl-ketimines were obtained the corresponding arylmethylidenecyanoacetic acids and the arylmethylideneacetonitriles, which are not accessible from the corresponding α-aryl ketones. PhHC:NBu and I (0.007 mole each) in 5 cc. absolute EtOH refluxed 5 min., cooled, diluted with Et2O, and filtered gave 90.2% BuNH2 salt of PhCH:C(CN)CO2H, (II), m. 115.5°, which was also obtained, m. 115-16°, from the free acid and the base in dry Et2O; the aqueous solution of the salt acidified with about N HCl gave II, m. 180° (uncor.) (all m.ps. are corrected except where stated otherwise). PhCH:NCH2CH2OH (2 g.) and 1.23 g. I in 60 cc. absolute EtOH stirred at 37°, diluted with Et2O, and filtered gave 100% HOCH2CH2NH2 salt of II, m. 151°, which was also prepared from the free acid and base, m. 151-2° (m. 157°); the salt in H2O acidified yielded 80% II, m. 180°. PhCH:NPh (0.865 g.) and 0.405 g. I in 5 cc. absolute EtOH refluxed 5 min. and cooled gave the PhNH2 salt, m. 132-3°, of II, which in H2O (acidified) gave 61.8% II; the salt, m. 135-6°, was also obtained from II and PhNH2. Furfurylideneaminoethanol (2.93 g.), 1.85 g. I, and 3 cc. absolute EtOH heated, cooled, and filtered yielded 100% yellowish H2NCH2CH2OH salt of furfurylidenecyanoacetic acid (III), m. 134.5°, which acidified in H2O gave 100% yellowish III, m. 222°. Furfurylideneaniline (2.71 g.) in 5 cc. hot absolute EtOH refluxed a few min. with 1.35 g. I and cooled, and the impure product treated with acid gave 9.7% III, m. 222°. o-ClC6H4CH:NBu (IV) (15.33 g.) and 7.00 g. I in 15-20 cc. absolute EtOH refluxed 10 min. gave 81.4 g. BuNH2 salt, m. 129°; the filtrate treated with NH3-MeOH and filtered, and the residual NH4 salt combined with the BuNH2 salt, dissolved in H2O, and treated with acid gave 88.2% o-ClC6H4CH:C(CN)CO2H, m. 205-7° (mixture of cis and trans isomers). p-Isomer of IV (13.9 g.), 7.0 g. I, and 15 cc. absolute EtOH gave similarly 83.8% BuNH2 salt of p-ClC6H4CH:C(CN)CO2H (V), m. 165°; the filtrate treated with NH3-MeOH, and the precipitate dissolved in boiling H2O and acidified with 2N HCl yielded 90.5% V. The BuNH2 salt added with stirring in portions to 300 cc. boiling H2O and treated with excess 2N HCl yielded 100% V, m. 200°. PhCH(N:CHPh)2 (0.80 g.) and 0.70 g. I in 25 cc. absolute EtOH refluxed a few min., cooled, and filtered yielded 92.5% NH4 salt of II, m. 203°; the filtrate concentrated, diluted with H2O, and filtered gave 61% II, m. 179-80°; the NH4 salt in hot H2O acidified yielded 94% II. Hydrofuramide (1.065 g.) in 10 cc. hot absolute EtOH treated with 1.01 g. I in 5 cc. hot absolute EtOH, heated 10-15 min., and cooled gave a mixture of the NH4 salt of furfurylidenecyanoacetic acid (VI) and II; the purified NH4 salt m. 184°; the filtrate evaporated, and the residue dissolved in H2O and acidified yielded 41.7% yellow VI, m. 218-21°; the NH4 salt yielded

L6 ANSWER 130 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

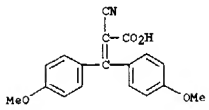
97.3% VI, m. 218°. p-ClC6H4CH(N:CHC6H4Cl-p)2 in hot abs. EtOH treated with I, dild. with Et2O, and filtered gave 73.6% NH4 salt of p-ClC6H4CH:C(CN)CO2H (VII), which yielded in the usual manner 74.7% VII, m. 200-2°. 3,4-(MeO)2C6H3CH[N:CHC6H3(OMe)2-3,4]2 (1.14 g.), 0.7 g. I, and 25 cc. abs. EtOH refluxed a few min., cooled, and dild. with Et2O pptd. 95.3% NH4 salt of 3,4-(MeO)2C6H3CH:C(CN)CO2H (VIII), m. 176.5°; the filtrate treated with NH3-MeOH gave 34% NH4 salt, which treated with acid yielded VIII, m. 241-2°. Ph2C:NH (IX) (18 g.) in dry Et2O treated with 8.5 g. I in Et2O, a portion of the pptd. oily IX-I salt dissolved in H2O, and the soln. allowed to stand gave BzPh; the remainder of the oily product treated in the presence of Et2O with concd. HCl, and the ppt. dissolved in H2O, heated to turbidity, and cooled deposited BzPh; the oily salt kept overnight at room temp. and heated a few min. yielded Ph2C:C(CN)CO2NH4 (X). IX and I (equimolar amts.) in Et2O-EtOH kept 2 months deposited X, m. 175°. IX (3.49 g.) and 1.645 g. I in 10 cc. abs. EtOH refluxed 0.5 hr., cooled, and filtered gave 81.3% X. X in H2O acidified with N HCl gave 85.5% Ph2C:C(CN)CO2H (XI), m. 212° (aq. EtOH). IX (0.55 g.) and 0.28 g. I heated under N to about 100° and then 2.5 hrs. at 180° gave 100% NH3 and Ph2C:CHCN, m. 46.5-47° (aq. EtOH). 9-Iminofluorene (0.96 g.) and 0.52 g. I in 10 cc. abs. EtOH refluxed a few min., cooled, and dild. with about 90 cc. Et2O gave 74.7% NH4 salt, m. 175-80° (decompn.), which treated in H2O with 0.1N HCl gave 78.2% fluorenylidenecyanoacetic acid, m. 214° (decompn.) (Et2O-petr. ether). EtPhCH:NH (3.7 g.) with 4 g. I yielded 56% EtPhC:C(CN)CO2H, m. 93°, which recrystd. several times gave 2 isomers, m. 91° and 129-30°. Ph2C:CHC:PhNH (2 g.) and 0.72 g. I in 5 cc. abs. EtOH refluxed 12 hrs., cooled, dild. with Et2O, and filtered, and the residual salt treated with refluxing 2N HCl yielded 16.3% Ph2C:CHCPh:C(CN)CO2H, m. 186°; the filtrate gave 6.5% of an isomer, m. 173°. Ph2C:NCH2CH2OH (3.48 g.) and 1.31 g. I in EtOH refluxed 24 hrs. and cooled yielded 62.4% H2NCH2CH2OH salt of Ph2C:C(CN)CO2H, m. 156°, which acidified in H2O yielded XI, m. 212°. EtPhC: NMe (XII) (7.42 g.) and 4.52 g. I in EtOH refluxed 1 hr., cooled, and dild. with Et2O gave 20.2% hygroscopic MeNH2 salt of EtPhC:C(CN)CO2H (XIII); the filtrate dild. with NH3-MeOH and a large amt. of Et2O, and the ppt. acidified in H2O gave XIII; the Et2O-EtOH filtrate washed with 0.1N aq. NaOH, and the alk. ext. acidified yielded XIII, m. 130°. (p-MeOC6H4)2C:NCH2Ph and I in EtOH refluxed 18 hrs. and worked up as for the acid gave the yellow (p-MeOC5H4)2C:C(CN)CO2H, m. 169° (aq. EtOH). XII (5.08 g.) and 3.42 g. I in EtOH refluxed 8 hrs. and evapd., and the residue heated with Cu powder under N gave 43.7% EtPhC:CHCN, b13 137°, b14 140-2°. PH2C:NPh refluxed 24 hrs. with excess I gave NCCH2CONHPh, m. 199°.

IT **20168-04-1**, Acrylic acid, 2-cyano-3,3-bis(p-methoxyphenyl)- (preparation of)

RN 20168-04-1 CAPLUS

CN 2-Propenoic acid, 2-cyano-3,3-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 130 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L6 ANSWER 131 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1964:3001 CAPLUS

DOCUMENT NUMBER: 60:3001

ORIGINAL REFERENCE NO.: 60:471c-h

TITLE: Alkylidene formation with imines and active methylene groups. I. Alkylidene derivatives of malononitrile

AUTHOR(S): Charles, George

CORPORATE SOURCE: Fac. Sci., Poitiers

SOURCE: Bulletin de la Societe Chimique de France (1963), (8-9), 1559-65
CODEN: BSCFAS; ISSN: 0037-8968

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

OTHER SOURCE(S): CASREACT 60:3001

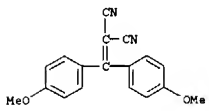
AB A series of alkylidenemalononitriles was prepared from appropriate ketimines, instead of the ketones, with CH2(CN)2 (I). The free ketimines, particularly the diarylketimines, were much more reactive towards I than the corresponding ketones. p-MeOC6H4CH:NBu (II) (1.88 g.) and 0.70 g. I heated under N at 90-100° (BuNH2 evolved), and the cooled residue recrystd. from EtOH yielded 11% p-MeOC6H4CH:C(CN)2 (III), m. 115° (all m.pp. are corrected, except where otherwise stated). I (0.8 g.) added to 2.10 g. II in 1 cc. AcOH and heated a little yielded 96.3% III. PhCH(N:CHPh)2 (0.165 g.) and 0.17 g. I fused over a small flame under N gave 86.5% NH3 and 82.5% PhCH:C(CN)2, m. 84.5° (aqueous EtOH). Hydrofuramide yielded similarly furfurylidenemalononitrile, m. 72° (red melt) (aqueous EtOH). Ph2C:NH (IV) treated with I (NH3 evolved) and worked up after a few min. gave nearly 100% Ph2C:C(CN)2 (V), m. 139° (EtOH), 141° (uncor.). I (0.98 g.) in 1.4 cc. AcOH and 2.65 g. IV yielded 96.7% V, m. 140°. IV.HCl and IV oxalate kept several weeks with excess I and then diluted with H2O yielded only BzPh. 9-Iminofluorene (1.80 g.) and 0.86 g. I in 10 cc. absolute EtOH yielded 100% 9-fluorenylidenemalononitrile, m. 237-5° (uncor.) (EtOH). Ph(p-MeC6H4)C:NH (1 g.) treated with 0.32 g. I (effervescence), heated with 2 cc. absolute EtOH, and cooled gave about 100% Ph(p-MeC6H4)C:C(CN)2, yellowish crystals, m. 108.5° (95% EtOH). (p-MeC6H4)2C:NH gave similarly about 100% yellow (p-MeC6H4)2C:C(CN)2, m. 131° (uncor.), resolidified (turning white) and remelting at 140.5° (uncor.). (p-Me2NC6H4)2C:NH (1 g.), 0.25 g. I, and 5 cc. absolute EtOH heated gave about 100% red-orange (p-Me2NC6H4)2C:C(CN)2, m. 245-5°. PH2C:CHC(:NH)Ph (2 g.) in 7 cc. hot absolute EtOH treated with 0.50 g. I, heated to reflux, cooled, and filtered gave about 100% yellow PH2C:CHCPh:C(CN)2, m. 148.5° (EtOH). Ph(m-ClC6H4)C:NH (1.67 g.) and 0.63 g. I in 3 cc. AcOH heated, diluted with a little absolute EtOH, and cooled yielded 90% Ph(m-ClC6H4)C:C(CN)2, m. 119.5° (absolute EtOH). EtPhC:NH (1.305 g.) (liberated from the acetate in Et2O with NH3 and evaporated) treated with I (effervescence) gave a min. of 65.2% EtPhC:C(CN)2, m. 68° (aqueous EtOH). Ph2C:NPh refluxed with I and filtered yielded Ph2C:C(CN)2, m. 141° (uncor.). PH2C:NCH2CH2OH (1.35 g.), 0.40 g. I, and 5 cc. absolute EtOH heated during 15 min. to reflux yielded 72.5% V, m. 141°; the filtrate acidified gave BzPh. (p-MeOC6H4)2C:NPh (1 g.) and 0.2 g. I in 2 cc. absolute EtOH refluxed a few min. gave about 100% (p-MeOC6H4)2C:C(CN)2, yellow solid, m. 153.5° (uncor.) (95% EtOH). Ph(Me3C)C:NBu (3.70 g.), 1.1 g. I, and a few cc. absolute EtOH gave similarly 52.8% Ph(Me3C)C:C(CN)2, m. 115.5° (95% EtOH). EtPhC:NBu (1.5 g.) and 0.55 g. I in EtOH refluxed 15 min. gave a min. of 45% EtPhC:C(CN)2, m. 68°.

IT **21453-19-0**, Malononitrile, [bis(p-methoxyphenyl)methylene]- (preparation of)

RN 21453-19-0 CAPLUS

L6 ANSWER 131 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

CN Propanedinitrile, [bis(4-methoxyphenyl)methylene]- (9CI) (CA INDEX NAME)

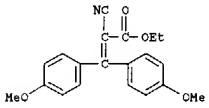


L6 ANSWER 132 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1963:481857 CAPLUS
DOCUMENT NUMBER: 59:81857
ORIGINAL REFERENCE NO.: 59:15147f-g
TITLE: Physical-chemical properties of some α-ethylenic acids and esters
AUTHOR(S): Guellec, Paulette Rivet-Le; Vandeven, Daniel; Carrie, Robert
CORPORATE SOURCE: Fac. Sci., Rennes, Fr.
SOURCE: Compt. Rend. (1963), 257(15), 2124-7
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

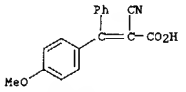
AB A study is made of the effect of X in (p-XC6H4)RCO (I) on the ionization consts. of the acids and the infrared spectra of the acids and esters obtained by condensation of I with NCCH2CO2Et (CA 56, 7208b). pK values obtained in 20% volume/volume aqueous EtOH ranged from 1.84 for I (X = NO2, R = XC6H4) to 3.02 for I (X = MeO, R = Me). Tables of frequencies at maximum absorption in the region 5.6-6 μ (C:O) (solution in CCl4 and suspension in Nujol), and 6-6.6 μ (C:C) (suspension in Nujol) are given. In general in a given series νC:O for the trans ester is shown to be a linear function of the pK of the corresponding acid.

IT **14442-41-2**, Acrylic acid, 2-cyano-3,3-bis(p-methoxyphenyl)-, ethyl ester **93325-33-8**, Cinnamic acid, α-cyano-p-methoxy-β-phenyl-
(ionization and spectrum of)

RN 14442-41-2 CAPLUS
CN 2-Propenoic acid, 2-cyano-3,3-bis(4-methoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)

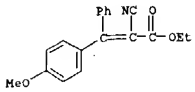


RN 93325-33-8 CAPLUS
CN Cinnamic acid, α-cyano-p-methoxy-β-phenyl- (7CI) (CA INDEX NAME)

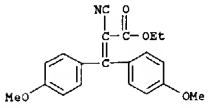


IT **14442-38-7**, Cinnamic acid, α-cyano-p-methoxy-β-phenyl-, ethyl ester **14442-41-2**, Acrylic acid, 2-cyano-3,3-bis(p-methoxyphenyl)-, ethyl ester
(spectrum of)

L6 ANSWER 132 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RN 14442-38-7 CAPLUS
CN 2-Propenoic acid, 2-cyano-3-(4-methoxyphenyl)-3-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



RN 14442-41-2 CAPLUS
CN 2-Propenoic acid, 2-cyano-3,3-bis(4-methoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 133 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1963:448137 CAPLUS
DOCUMENT NUMBER: 59:48137
ORIGINAL REFERENCE NO.: 59:8661e-f
TITLE: Diphenylmethylenemalonitriles
INVENTOR(S): Strobel, Albert F.; Catino, Sigmund C.
PATENT ASSIGNEE(S): General Aniline & Film Corp.
SOURCE: 23 pp.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
PATENT INFORMATION:

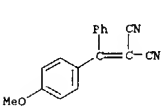
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 1320280		19630308	FR	
GB 974111			GB	
GB 992969			GB	
PRIORITY APPLN. INFO.:			US	19610323

GI For diagram(s), see printed CA Issue.

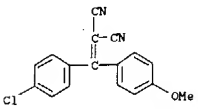
AB Compds. of the formula I, in which X, Y = H, halo, cyano, hydroxy, alkoxy, carboxy, sulfamido (but neither NO2 nor NH2) were prepared A mixture of 16.5 g. CH2(CN)2, 62.75 g. 4,4'-dichlorobenzophenone, 3.85 g. AcONH4, 12 mL. AcOH, and 75 mL. C6H6 was refluxed for 12 h. The C6H6 was distilled, 150 mL. H2O added, and the mixture filtered to yield I (X = Y = p-Cl), b0.5 185-200°. Similarly made were I (X and Y given): H, p-dodecyloxy; p-MeO, p-Cl; H, p-MeO; o-Cl, p-Cl; H, p-HOCH2- CH2(OCH2CH2)nO. In the following I, X = Y: p-OH; p-PhSO2O. These compds. are UV absorbers. Procedures to incorporate them, preferably 0.5-2%, into cellulose acetate, natural and synthetic waxes, and other polymers, are given.

IT **17212-45-2**, Malononitrile, (p-methoxy-α-phenylbenzylidene)-, **93261-79-1**, Malononitrile, [p-chloro-α-(p-methoxyphenyl)benzylidene]-
(preparation of)

RN 17212-45-2 CAPLUS
CN Propanedinitrile, [(4-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)



RN 93261-79-1 CAPLUS
CN Malononitrile, [p-chloro-α-(p-methoxyphenyl)benzylidene]- (7CI) (CA INDEX NAME)



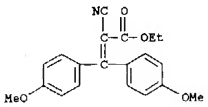
L6 ANSWER 133 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

L6 ANSWER 134 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1963:39492 CAPLUS
DOCUMENT NUMBER: 58:39492
ORIGINAL REFERENCE NO.: 58:6666c-e
TITLE: Syntheses and physical chemical studies of substituted ethyl 2-cyano-2-propenoates and their derivatives. III. Kinetic study of the hydrolysis and nitrilation of the ethyl 2-cyano-2-propanoates
AUTHOR(S): Carrie, Robert
CORPORATE SOURCE: Univ. Rennes, Fr.
SOURCE: Bulletin de la Societe Scientifique de Bretagne (1962), 37, 59-98
CODEN: BSSBAS; ISSN: 0037-9581
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Spectrophotometric measurements (ultraviolet spectra) were made during the hydrolysis and nitrilation of I. Various esters were hydrolyzed with alc. KOH and the rate consts. for the formation of the aldehyde or ketone and cyanoacetic acid from the ethylenic acids were determined (R, (R', k + 10-3 min.-1 given): 4-ClC6H4, Me, 28; Ph, H, --; Ph, Me, 13.2; Ph, Ph, 1.35; 4-O2NC6H4, 4-O2N-C6H4, 95.4; 4-MeOC6H4, 4-MeOC6H4, 0.542; Ph, PhCH2, --; PhCH2, PhCH2, -- I (R = 4-XC6H4, R' = Me) (X given): NO2, 114.5; Me, 10.7; MeO, 12.2. The above studies were made at 30°. I were hydrolyzed and simultaneously nitrilated to the corresponding 3,3-disubstituted-2,3-dicyanopropanoates (hydrolysis reaction rate constant + 103 min.-1, nitrilation reaction rate constant + 103 min.-1 given: R = Ph, R' = H, 230, 800; R = 4-XC6H4 (X = NO2), R' = Me (m.p. 144°), 15.7, 80.5, and (m.p. 93-4°), --, 71; X = Cl (m.p. 88°), 12.8, 57; X = MeO (solid), 5.65,25.3; R = R' = Ph, --, 7.8; R = Ph, R' = Me (m.p. 46-7°), 12.0, 44, and (oil), --, 51.

IT **14442-41-2**, Acrylic acid, 2-cyano-3,3-bis(p-methoxyphenyl)-, ethyl ester
(hydrolysis of, kinetics of)

RN 14442-41-2 CAPLUS
CN 2-Propenoic acid, 2-cyano-3,3-bis(4-methoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)



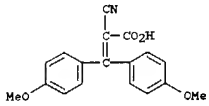
L6 ANSWER 135 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1962:38285 CAPLUS
DOCUMENT NUMBER: 56:38285
ORIGINAL REFERENCE NO.: 56:7208b-f
TITLE: The preparation and hydrolysis of some substituted ethyl 2-cyano-3,3-diphenyl-2-propenoates, dinitriles, nitrile amides, and the corresponding unsubstituted diesters
AUTHOR(S): Carrie, Robert; Bargain, Michel
CORPORATE SOURCE: Univ. Rennes, Fr.
SOURCE: Compt. Rend. (1961), 253, 1962-4
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB Substituted benzophenones condensed with NCCH2CO2Et by the method of Dufraisse, et al. (CA 46, 2533c), yielded the corresponding XC6H4(X'C6H4)C:C(CN)CO2Et (I); the monosubstituted I were obtained as the geometric isomers. In this manner were prepared the following I (X, X', % yield, and m.p. of isomers given): NO2, H, 90, 140°, 94°; Cl, H, 84, 113°, 84°; MeO, H, 81, 79-81°, 63-4°; NO2, NO2, 75, 100-2°, -; Cl, Cl, 65, 84°, -; MeO, MeO, 82, 93°, -. The appropriate I refluxed 45 min. with aqueous alc. N Na2CO3 gave the corresponding XC6H4(X'C6H4)C:C(CN)CO2H (X, X', % yield, and m.p. given): NO2, H (monohydrate), 66, 96°; Cl, H, 80, 172°; MeO, H, 79, 160°; NO2, NO2, 52, 254-7°, Cl, Cl (monohydrate), 77, 108°; MeO, MeO, 78, 165°. The condensation of benzophenone with CH2(CN)2 and NCCH2CONH2 gave Ph2C:C(CN)2 (II) and Ph2C:C(CN)CONH2 (III), resp., which (both) saponified with aqueous alc. Na2CO3 yielded 100% BzPh. II with aqueous alc. KCN yielded Ph2C(CN)CH(CN)2 (IV). III gave similarly IVa, m. 162°. IV heated with aqueous alc. N Na2CO3 was converted quant. to BzPh. Ph2C:C(CO2Et)2 (V) refluxed 3.5 hrs. with aqueous alc. N Na2CO3 yielded 58% Ph2C:C(CO2Et)CO2H (VI), m. 144°. VI heated at 240-50° gave Ph2C:CHCO2Et, which (saponified) yielded Ph2C:CHCO2H. V refluxed 1.5 hrs. with aqueous alc. NaOH gave 100% Ph2C:C(CO2H)2.

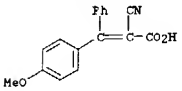
IT **20168-04-1**, Acrylic acid, 2-cyano-3,3-bis(p-methoxyphenyl)-
93325-33-8, Cinnamic acid, α-cyano-p-methoxy-β-phenyl-
(preparation of)

RN 20168-04-1 CAPLUS
CN 2-Propenoic acid, 2-cyano-3,3-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



RN 93325-33-8 CAPLUS
CN Cinnamic acid, α-cyano-p-methoxy-β-phenyl- (7CI) (CA INDEX NAME)

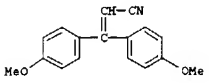
L6 ANSWER 135 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



L6 ANSWER 136 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1959:77724 CAPLUS
DOCUMENT NUMBER: 53:77724
ORIGINAL REFERENCE NO.: 53:14066i,14067a-f
TITLE: Preparation of diaryl β-hydroxyamides and nitriles; dehydration to the corresponding α-ethylenic derivatives
AUTHOR(S): Chodkiewicz, Wladyslaw; Cadiot, Paul; Willemart, Antoine; Prevost, Sylviane
SOURCE: Bulletin de la Societe Chimique de France (1958) 1586-91
CODEN: BSCFAS; ISSN: 0037-8968
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 53:77724

AB ArAr'C:O (0.01 mole) added to a mixture at 0° of RCH2X (slight excess for nitriles, 3 to 4 moles per mole ketone for amides or sulfonamides), pulverized anhydrous KOH (4 moles per mole ketone for nitriles, 8 for amides and sulfonamides), and a solvent (Et2O, tetrahydrofuran of HCONMe2), a large amount of H2O added after the thermal reaction subsided (2-10 min.) and the product extracted gave ArAr'C(OH)CHRX which on boiling with 2% H2SO4 was dehydrated to ArAr'C:CRX. The following compds. were prepared (reaction solvent, time of reaction in min., crystallizing solvent, m.p., and % yield of alc., and time of reaction, crystallizing solvent, m.p., and yield of the corresponding unsatd. compound given): 1,1-diphenyl-2-cyanoethanol (I) and -ethene, Et2O, 5, C6H6-ligroine, 140° (b18, 202-4°), 95, 1, MeOH, 45°, 94; 1,1-biphenylene-2-cyanoethanol (II) and -ethene, Et2O, 5, C6H6, 110°, 91, 0.5, MeOH, 110°, 95; 1-phenyl-1-(p-tolyl)-2-cyanoethanol and -ethene, Et2O, 10, C6H6-C6H12, 137°, 78, 0.5, -, - (b18 204-7°), 94; 1,1-bis(p-bromophenyl)-2-cyanoethanol and -ethene, Et2O, -, CCl4-ligroine, 138°, 88, 1, H2O-EtOH, 102°, 92; 1,1-bis(p-methoxyphenyl)-2-cyanoethanol and ethene, Et2O, -, CCl4-ligroine, 100°, 84, 0.5, 75% EtOH, 112°, 95; 1-phenyl-1-(β-naphthyl)-2-cyanoethanol and -ethene, Et2O, 5, PhMe-C6H12, 168°, 93, 0.5, EtOH, 90°, 85; 2-phenyl-3,3-dimethyl-1-cyano-2-butanol (cannot be dehydrated), tetrahydrofuran, 5, ligroine, 101°, 75; 1,1,3-triphenyl-4-cyano-1-buten-3-ol (not dehydrated), tetrahydrofuran, 30, ligroine, 110°, 60; 1,1-diphenyl-2-methyl-2-cyano-1-propanol and 1-propene, Et2O, 15, PhMe-ligroine, 126°, 79, 5, ligroine, 63°, 70; 1,1-diphenyl-2-ethyl-2-cyano-1-butanol and -1-butene, -, 15, PhMe, 164°, 38, 2, petr. ether-ligroine, 76°, 72; 1,1,2-triphenyl-2-cyanoethene (alc. not isolated), tetrahydrofuran, 1 hr., ligroine, 166°, 25; 2-dimethylcarbamoylethanol (III) and -ethene, -, 10, C6H6-ligroine, 96° (resolidified and m. 104°), 45, 0.5, CCl4-Et2O, 80°, 89; 2-dimethylcarbamoyl-1,1-biphenylenethanol (IV) (no dehydration), -, 5 at -5-10°, CCl4-C6H12, 70°, 82; 2-diethylcarbamoyl-1,1-diphenylethanol and -ethene, -, 10, PhMe, 88°, 50, 2, ligroine, 83°, 74; 2-methylphenylcarbamoyl-1,1-diphenyl-N-methylethanol (no dehydration), HCONMe2, 15 CCl4-C6H12, 108°, 27°; 4-(3-hydroxy-3,3-diphenylpropinyl)morpholine and 4-(3,3-diphenylpropenoyl)morpholine, -, 10, PhMe, 150°, 50, 2, C6H12, 100°, 65; 3-(hydroxydiphenylmethyl)-1-methyl-2-pyrrolidone (V) and 3-(diphenylmethylene-)1-methylpyrrolidone, -, 10, CCl4-ligroine, 85° (resolidified, new m.p. 99°), 89, 2, CCl4-ligroine, 117°, 87; 3-(9-hydroxy-9-fluorenyl)-1-methyl-2-pyrrolidone (VI) and 3-(9-fluorenylidene)-1-methyl-2-pyrrolidone, -, 15, PhMe, 175°, 77, 2, PhMe-ligroine, 173°, 88; 2-dimethylsulfamoyl-1,1-diphenylethanol and the corresponding ethene, Et2O, 15, C6H6, 96°, 25, 2-3, MeOH-H2O, 144°, 84. The alcs. react under the reaction conditions

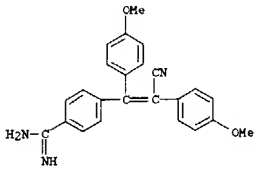
L6 ANSWER 136 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
for ethynylation (C.A. 50, 6308d; 52, 14565c) with PhC.tplbond.CH or HC.tplbond.CCH2OH to regenerate RCH2X and give the following % yields of ArAr'C(OH)C.tplbond.CPh and ArAr'C(OH)C.tplbond.CCH2OH resp.: I, 97, 52; II, 85, 44; III, 98, 94; IV, 98, 77; V, 98, 90; VI, 98, 64. This proves the reversibility of these reactions and justifies in part the use of disubstituted amides as solvents in the ethynylation reaction.
IT **101441-96-7**, Acrylonitrile, 3,3-bis(p-methoxyphenyl)-
(preparation of)
RN 101441-96-7 CAPLUS
CN 2-Propenenitrile, 3,3-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)



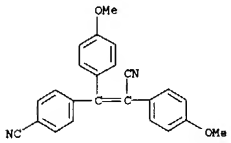
L6 ANSWER 137 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1959:56302 CAPLUS
DOCUMENT NUMBER: 53:56302
ORIGINAL REFERENCE NO.: 53:10134b-c
TITLE: 5,5'-Dinitro-2,2'-dichlorobenzil
INVENTOR(S): Moureu, Henri; Chovin, Paul
PATENT ASSIGNEE(S): Societe des usines chimiques de Rhone-Poulenc
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 807985		19590128	GB	

AB See U.S. 2,824,899 (C.A. 52, 12916b).
IT **102664-69-7**, Benzamidine, p-[2-cyano-1,2-bis(p-methoxyphenyl)vinyl]- **102755-63-5**, α,4'-Stilbenedicarbonitrile, 4-methoxy-α'-(p-methoxyphenyl)- **124105-52-8**, Benzimidic acid, p-[2-cyano-1,2-bis(p-methoxyphenyl)vinyl]-, ethyl ester, dihydrochloride
(preparation of)
RN 102664-69-7 CAPLUS
CN Benzamidine, p-[2-cyano-1,2-bis(p-methoxyphenyl)vinyl]- (6CI) (CA INDEX NAME)

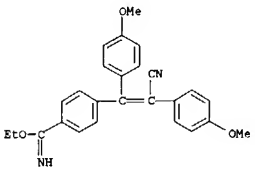


RN 102755-63-5 CAPLUS
CN α,4'-Stilbenedicarbonitrile, 4-methoxy-α'-(p-methoxyphenyl)- (6CI) (CA INDEX NAME)



L6 ANSWER 137 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 124105-52-8 CAPLUS
CN Benzimidic acid, p-[2-cyano-1,2-bis(p-methoxyphenyl)vinyl]-, ethyl ester, dihydrochloride (6CI) (CA INDEX NAME)



●2 HCl

L6 ANSWER 138 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1959:56301 CAPLUS
DOCUMENT NUMBER: 53:56301
ORIGINAL REFERENCE NO.: 53:10133e-i,10134a-b
TITLE: Substituted 1,1,2-triphenylethylenes
PATENT ASSIGNEE(S): Wm. S. Merrell Co.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

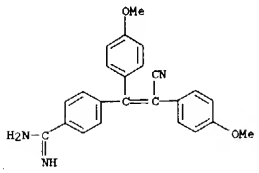
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 797345		19580702	GB	

AB 1,1-Di-p-anisyl-2-cyanophenylethylene (prepared from the corresponding halo compound by reaction with CuCl2) (27.2 g.) in 38 ml. anhydrous EtOH and 500 ml. dry C6H6 is saturated with HCl at 5° and allowed to stand 3 days, the solvent evaporated, and the residue triturated with Et2O to form 1,1-dianisyl-2-(p-ethoxycarbiminophenyl) ethylene HCl salt (I), yellow, m. 131° (decomposition). Hydrochlorides of 1-(p-anisyl)-1-(o-anisyl)-2-(p-ethoxycarbiminophenyl)ethylene has an indefinite m.p., indicating stereoisomers. Similarly are formed: 1,1-di-m-anisyl-2-(p-ethoxycarbiminophenyl)ethylene; 1,2-di-p-anisyl-1-(m-ethoxycarbiminophenyl)ethylene (II), m. 119-20° (decomposition); 1,1-di-p-anisyl-2-(m-ethoxycarbiminophenyl)ethylene (III), m. 140° (decomposition); 1,2-di-p-anisyl-1-(p-ethoxycarbiminophenyl)ethylene, m. 118-20° (decomposition); 1,2-diphenyl-1-(m-ethoxycarbiminophenyl)ethylene (IV) isomeric imidoester HCl salts, m. 142° and 117°, resp. (both decomposition); 1,1-di-p-tolyl-2-(p-ethoxycarbiminophenyl)ethylene, m. 148° (decomposition). I (13.5 g.) is suspended in 100 ml. CHCl3, poured over 160 g. cracked ice, neutralized with 30% NaOH to pH 8, the CHCl3 layer separated, dried over Na2SO4 at 0°, the residue after evaporation of CHCl3 dissolved in 65 ml. EtOH solution, heated to 60°, treated with 2.50 g. NH4Cl (V) in 5 ml. H2O, chilled 6 hrs. then filtered, and the filtrate evaporated to 25 ml. to yield 1,1-di-p-anisyl-2-(p-guanylphenyl)ethylene HCl salt (VI), m. 252-6° (decomposition). II yields 1,1-di-p-anisyl-2-(m-guanylphenyl)ethylene HCl salt (VII), m. 232-3°. The lower melting isomer yields 1,2-diphenyl-1-(m-guanylphenyl)ethylene-HCl (VIII), m. 234-7°. The higher melting isomer yields VIII, m. 237.5-8.5°. Under similar conditions H2N(CH2)2NH2, 1,3-diaminopropane, piperidine (IX), separately may replace V and yield, resp., 1,1-di-p-anisyl-2-(p-2-imidazolinylphenyl)ethylene HCl salt (X), m. 261-2°, from a hot mixture of EtOH 50, MeCOEt 100, petr. ether (b. 75-90°) 25 parts. 1,1-Di-p-anisyl-2-[p-(1,4,5,6-tetrahydropyrimidinyl)phenyl] ethylene HCl salt m. 238-40°; 1,1-di-p-anisyl-2-(p-piperidinocarbiminophenyl)ethylene HCl salt m. 150° (decomposition). Pyrrolidine or morpholine may replace IX. A mixture of 4.0 g. NaOH in 16 ml. H2O, 20 g. VI, and 6.7 g. MeCOCH2CO2Et in 60 ml. EtOH is allowed to stand at room temperature 4 days then the solvent removed, the residue dissolved in CHCl3, the solution washed H2O, dried with Na2SO4, the solvent removed, and the residue titrated with Et2O to yield 11.2 g. 1,1-di-p-anisyl-2-[p-(4-methyl-6-hydroxy-2-pyrimidinyl)phenyl] ethylene, yellow prisms, m. 217-18° (EtOH-CH2Cl2). Br (16 g.) in 200 ml. CCl4 (XI) is added to 34 g. 1-(p-cyanophenyl)-1,2-di-p-anisylethylene (m. 122-3°) in 4 hrs., XI removed, the residue dissolved in 200 ml. dry C5H6N, 9 g. CuCl2 added to the solution, the mixture refluxed 6 hrs. then poured into 1000 ml. cold concentrated HCl, and extracted with CHCl3. The exts. dried over MgSO4 and the solvent removed yield

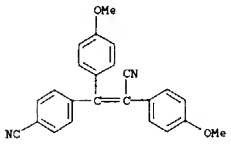
L6 ANSWER 138 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
3-(p-cyanophenyl)-2,3-di-p-anisylacrylonitrile (XII). XII may be converted to the corresponding 3-(p-ethoxycarbiminophenyl)-2,3-di-p-anisylacrylonitrile di-HCl salt (XIII), yellow, and XIII in turn to yellow 3 -(p - guanylphenyl) - 2,3 - dianisylacrylonitrile. These compds. have the following activities: II, VIII, and X antiinflammatory and antigranuloma; II, III, and VIII eosinopenic, II and X antifungal.

IT **102664-69-7**, Benzamidine, p-[2-cyano-1,2-bis(p-methoxyphenyl)vinyl]- **102755-63-5**, α,4'-Stilbenedicarbonitrile, 4-methoxy-α'-(p-methoxyphenyl)- **124105-52-8**, Benzimidic acid, p-[2-cyano-1,2-bis(p-methoxyphenyl)vinyl]-, ethyl ester, dihydrochloride
(preparation of)

RN 102664-69-7 CAPLUS
CN Benzamidine, p-[2-cyano-1,2-bis(p-methoxyphenyl)vinyl]- (6CI) (CA INDEX NAME)

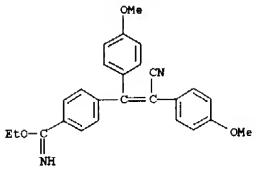


RN 102755-63-5 CAPLUS
CN α,4'-Stilbenedicarbonitrile, 4-methoxy-α'-(p-methoxyphenyl)- (6CI) (CA INDEX NAME)



RN 124105-52-8 CAPLUS
CN Benzimidic acid, p-[2-cyano-1,2-bis(p-methoxyphenyl)vinyl]-, ethyl ester, dihydrochloride (6CI) (CA INDEX NAME)

L6 ANSWER 138 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)



●2 HCl

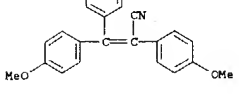
L6 ANSWER 139 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1957:92992 CAPLUS
DOCUMENT NUMBER: 51:92992
ORIGINAL REFERENCE NO.: 51:16880h-i,16881a
TITLE: The estrogenic action of new triphenylcyanoethylene derivatives
AUTHOR(S): Nishizuka, Yasuaki; Nakagawa, Kiyoshi; Tsujii, Yasushige; Kimura, Kiyoichi; Sakai, Kunio; Shimizu, Katsuhiko
CORPORATE SOURCE: Kyoto Univ. Med. School
SOURCE: Nippon Naibumpi Gakkaishi (1957), 33, 340-5
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB With 10 compds. the estrogenic action was estimated by subcutaneous injection of the compds. into ovariectomized mice (about 50 days old) on the 16th day after the operation. This was followed by Allen-Doisy's microscopic examination of vaginal epithelial cells for as long as 2 weeks. The results were as follows (M.D. and acting time as average of 3 mice are given): α-(p-methoxy-phenyl)-β,β-diphenylacrylonitrile, 5 γ, 3-4 days; α-(p-methoxyphenyl)-β,β-diphenylacrylic acid, 5 γ, 2-3 days; α,β,β-tris(methoxyphenyl)acrylonitrile, 10 γ, 4-6 days; α,-β,β-triphenylacrylonitrile, 50 γ, 2-3 days; α-(p-methoxy-m-tolyl)-β,β-diphenylacrylonitrile, 300 γ, 5-7 days; α,β,β-tris(p-methoxy-m-tolyl)acrylonitrile, 1 mg.; α-(p-methoxy-phenyl)-β,β-(p-tolyl)acrylonitrile, α-(p-nitrophenyl)-β,β-di-phenylacrylonitrile, α-(p-methoxyphenyl)-β,β-biphenyl-eneacrylonitrile, α-phenyl-β,β-biphenyleneacrylonitrile, >1 mg. With the compds. possessing estrogenic action a morphological examination of adrenal gland was carried out.

IT **35364-39-7**, Acrylonitrile, tris(p-methoxyphenyl)-
(estrogenic action of)

RN 35364-39-7 CAPLUS
CN Benzeneacetonitrile, α-[bis(4-methoxyphenyl)methylene]-4-methoxy- (9CI) (CA INDEX NAME)



L6 ANSWER 140 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1957:12698 CAPLUS
DOCUMENT NUMBER: 51:12698
ORIGINAL REFERENCE NO.: 51:2665d-g
TITLE: Preparation of β-hydroxy diarylamides and β-hydroxy diarylnitriles
AUTHOR(S): Chodkiewicz, Wladyslaw; Cadiot, Paul
SOURCE: Compt. rend. (1956), 243, 280-3
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Diaryl ketones have been condensed with N,N-disubstituted amides and with acetonitrile (I) in the presence of anhydrous potash to give βhydroxy diarylamides and β-hydroxy diarylnitriles. For the amides, it was necessary to use 8 moles potash/mole amide and for the nitriles 3-4 moles potash/mole nitrile. The reaction was rapid and exothermic. The hydroxy compds. have been dehydrated by heating in acid mediums (HOAc and H2SO4) to the ethylenic amides and nitriles in high yields. The following condensations have been carried out: Ph2CO and I give 95% product, m. 140°, which on dehydration gave 91% product, m. 45; fluorenone and I gave 91% product, m. 110° dehydration product (95%), m. 110°; p-MeC6H4COPh and I, 78% product, m. 137°, dehydration product (94%), b18 204-7°; di(p-MeOC6H4)2CO and I, 84% product, m. 100° dehydration product (95%), m. 112°; (p-BrC6H4)2CO and I, 88% product, m. 138°, dehydration product (92%), m. 102°; 2-C10H7COPh and I, 93% product, m. 168°, dehydration product (85%), m. 90°; Ph2CO and AcNMe2, 40% product, m. 96°, resolidifies and m. 104°, dehydration product (89%), m. 80°; Ph2CO and N-methylpyrrolidone, 89 % product, m. 85°, dehydration product (87%), m. 117°; fluorenone and N-methylpyrrolidone, 77% product, m. 175°, dehydration product (81%), m. 173°; and Ph2CO and MeSO2NMe2, 40% product, m. 96 °.

IT **101441-96-7**, Acrylonitrile, 3,3-bis(p-methoxyphenyl)-
(preparation of)

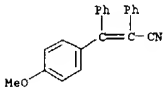
RN 101441-96-7 CAPLUS
CN 2-Propenenitrile, 3,3-bis(4-methoxyphenyl)- (9CI) (CA INDEX NAME)

L6 ANSWER 141 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1954:60341 CAPLUS
DOCUMENT NUMBER: 48:60341
ORIGINAL REFERENCE NO.: 48:10677a-g
TITLE: Antimitotic activity of substituted α-phenylcinnamic nitriles [1;2-diphenylvinyl cyanides]
AUTHOR(S): Lettre, Hans; Haede, Werner; Schafer, Lotti
SOURCE: Hoppe-Seyler's Zeitschrift fuer Physiologische Chemie (1952), 289, 298-309
CODEN: HSZPAZ; ISSN: 0018-4888
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 48:60341

AB 1;2-Diphenylvinyl cyanides are described carrying MeO, MeS, Me, NO2, Br, NMe2, and quaternary N substituents, together with some products of hydrogenation or hydrolysis. Reaction of CH2PhCN (I) with the appropriate benzaldehydes in EtOH-NaOH affords the following: 2-2';3'-dimethoxy-, C17H15O2N, m.p. 84°, 2-3'-bromo-4',5'-dimethoxy-, m.p. 99°, 2-2'-bromo-4',5'-dimethoxy-, C17H14O2NBr, m.p. 116°, 2-4'-methylthio-, C16H13NS, m.p. 97°, and 2-4'-nitrophenyl-1-phenylvinylcyanide, m.p. 120° (lit., 117-118°) (improved prepare in MeOH-NaOMe at -10° to 0°). From I (2 mol.) and p-CHOC6H4OMe in EtOH-NaOEt are obtained, 1-phenyl-2-p-methoxyphenylvinyl cyanide (II) and 1,3-diphenyl-2-p-methoxy-phenyl-1,3-dicyanopropane, C24H20ON2, m.p. 164-165°. p-C6H4BzOMe and I with NaNH2 yields 1,2-diphenyl-2-p-methoxy-phenylvinyl cyanide, C22H17ON, m.p. 137-138°. Addition of I and then p-OMeC6H4 CH2Cl to NaNH2 in Et2O, refluxing (15 min.) and treatment with H2O gives 1-phenyl-2-p-methoxyphenylethyl cyanide, C16H15ON (III), m.p. 86-87°. Reduction of II by Na-Hg in EtOH at room temperature affords III and 1-phenyl-2-p-methoxyphenylethane-1-carbonamide, C16H17O2N, m.p. 162° (main product at higher temperature), and hydrogenation of II (PtO2-AcOH) yields 2-phenyl-3-p-methoxyphenylpropylamine (hydrochloride, m.p. 164°). Hydrolysis of 1-phenyl-2-p-dimethylaminophenylvinyl cyanide (IV) (ethiodide, m.p. 169-170°) with H2SO4 at 100° for 3 hr., then room temperature overnight, affords 1-phenyl-2-p-dimethylaminophenylethylene-1-carbonamide, C17H18ON2, m.p. 230° (decomposition), and reduction of I (Na-Hg in EtOH under reflux) gives 1-phenyl-2-p-dimethylaminophenylethyl cyanide, C17H15N2, m.p. 76°, and 1-phenyl-2-p-dimethylaminophenylethane-1-carbonamide, C17H20ON2, m.p. 167°. Similar reduction (room temperature, 8 hr., then 80°, 1 hr.) of the following quaternary salts of IV affords tert-amine derivative (% in parenthesis): methosulphate (7.8%), benzyl iodide, m.p. 181° (86%) (chloride, m.p. 185-187°), allyl bromide, m.p. 191-192° (decomposition) (83%), and cinnamyl bromide, m.p. 185-187° (90%). The allyl derivative is not reduced to tert-amine by yeast. BzO2H and IV in C6H6 give the N-oxide, C17H16ON2, m.p. 147-148° (picrate, C17H16ON2.C6H3O7N3, m.p. 148°), which is reduced by Sn-HCl to IV. 1-Phenyl-2-p-aminophenylvinyl cyanide diazotized and reacted with PhNH.N:CHMe-aqueous NaOAc affords phenyl-p-(2-cyano-2-phenylvinyl)phenylformazylmethane, C23H19N5, m. p. 188°, which with Pb(OAc)4 in CHCl3 and then MeOH-HCl yields 2-phenyl-3-p-(2'-cyano-2'-phenylvinyl)phenyl-5-methyltetrazolium chloride, m.p. 237°.

IT **35363-69-0**, Acrylonitrile, 3-(p-methoxyphenyl)-2,3-diphenyl- (preparation of)

L6 ANSWER 141 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
RN 35363-69-0 CAPLUS
CN Benzeneacetonitrile, α-[(4-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)



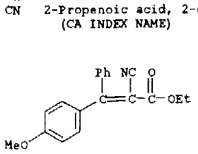
L6 ANSWER 142 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1953:54978 CAPLUS
DOCUMENT NUMBER: 47:54978
ORIGINAL REFERENCE NO.: 47:9348c-f
TITLE: Substituted cyanoacetates
INVENTOR(S): Cragoe, Edward J., Jr.
PATENT ASSIGNEE(S): Sharp & Dohme, Inc.
DOCUMENT TYPE: Patent
LANGUAGE: Unavailable
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2623060		19521223	US	

AB Compds. of the type R2C:C(CN)CO2R', where R are the same or different alkyl, aryl, alkaryl, or heterocyclic radicals, and R' is an alkyl group, were prepared by the Knoevenagel condensation of NCCH2CO2Et(I) with a suitable ketone, but with the NH4OAc(II) catalyst added in portions at intervals. Thus I 103, 2,4'-dichlorobenzophenone 190.2, HOAc 36.5 g., and C6H6 150 ml. were refluxed 92 hrs., in a flask connected to a Dean-Stark H2O separator, with 50 g. II added in small portions (2-3 g.) at 4-hr. intervals and the formed H2O layer removed before each addition, the mixture was cooled, washed with three 200-ml. portions of H2O, dried over Na2SO4, the C6H6 distilled, and the residue fractionated, giving 107.2 g. (41%) ethyl (2,4'-dichlorobenzhydrylidene)cyanoacetate, b0.1 168-85°, m. 105-6° (from EtOH). The following Et cyanoacetates were similarly prepared (α-substituent and % yield given): 4-methoxybenzhydrylidene, 75, b0.08 187-97°; [phenyl(2-thienyl)methylene], 49, b0.2 150-86°, m. 77-8° (from aqueous EtOH, then cyclohexane); 9-fluorenylidene, 76, b0.1 194-6°, m. 58-60°; diphenethylmethylene, 68, b0.25 187-92°, nD25 1.5567; (6-cyclohexyl-1-phenylhexylidene), 67, b0.1 190-5°, nD25 1.5260; benzhydrylidene, 84, b1-2 170-80°, m. 95-7° (from n-heptane); 2-camphanylidene, 37, b0.05 125-7°, m. 85.5-6.5° (from aqueous EtOH); and 3,3-dimethyl-2-butylidene, 13, b12 127-30°, nD25 1.4680.

IT **14442-38-7**, Cinnamic acid, α-cyano-p-methoxy-β-phenyl-, ethyl ester (preparation of)

RN 14442-38-7 CAPLUS
CN 2-Propenoic acid, 2-cyano-3-(4-methoxyphenyl)-3-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



L6 ANSWER 143 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1952:8572 CAPLUS
DOCUMENT NUMBER: 46:8572
ORIGINAL REFERENCE NO.: 46:1529i,1530a-i,1531a-b
TITLE: Some anthracene derivatives of potential biological interest
AUTHOR(S): Buu-Hoi, Ng. Ph.; Hoan, Ng.
CORPORATE SOURCE: Univ. Paris
SOURCE: Journal of Organic Chemistry (1951), 16, 874-81
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.

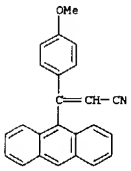
AB Because some simple anthracene derivs. (I), such as 9,10-dimethylanthracene (II) and 2-anthramine, have been found to be carcinogenic, some I are synthesized. 9-Anthraldehyde (III), prepared in 85% yield according to Fieser, et al. (C.A. 34, 5075.9), is converted into the thiosemicarbazone, fine yellow needles, m. 217°. Reduction of 100 g. III with 150 g. NZH4.H2O, and 120 g. KOH in 350 cc. (CH2OH)2 gives 97.7% 9-methylanthracene (IV), b13 198-202°. Cautiously adding 130 g. POCl3 to 90 g. IV, 127 g. PhNMeCHO, and 90 cc. o-C6H4Cl2, heating the mixture 1.5 h. on a water bath, pouring the cooled mixture into 1 l. H2O containing 200 g. NaOAc, removing the solvent by steam-distillation, and crystallizing the washed (6 N HCl, H2O, dilute NaOAc) precipitate from AcOH give 62 g. 9-methyl-10-anthraldehyde (V), shiny orange needles, m. 173° (semicarbazone, fine orange-yellow needles, m. above 350°; thiosemicarbazone, orange-yellow needles, softens with discoloration above 218°, m. 230°). Gradually heating at 200° with removal of H2O 30 g. V, 50 g. 85% NZH4.H2O, 50 g. KOH, and 250 cc. (CH2OH)2, refluxing the mixture until the thick orange-red froth formed has disappeared, diluting the mixture with H2O, and extracting with CHCl3 give over 90% II, large shiny yellow leaflets, m. 188°. Adding in small portions 32 g. III to PhCH2MgCl from 20 g. PhCH2Cl in 150 cc. ether, refluxing the mixture 0.5 h., treating the cold mixture with dilute H2SO4, and distilling the residue of the washed (H2O) and dried organic layer give 7 g. 9-styrylanthracene, b13 280°, large pale yellow leaflets, m. 226°, giving an orange-red color with H2SO4, and 21 g. of an isomer, C22H16, b13 280-300°, shiny pale yellow leaflets, m. 132°, which gives the same color with H2SO4. Adding 4.5 g. V to PhCH2MgCl from 5.5 g. PhCH2Cl gives 9-methyl-10-styrylanthracene, b13 300-10°, long orange needles, m. 157°, giving a pink color with H2SO4. Refluxing 3 g. III and 4 g. α-picoline in 10 g. Ac2O 48 h., adding dilute HCl to the cooled mixture, and treating the precipitate with hot 20% NaOH give 2 g. 1-(9-anthryl)-2-(2-pyridyl)ethylene, shiny greenish yellow needles, m. 215°, easily sublimable above 180°, giving an orange-red color with H2SO4. In the same way, 3 g. III and 4.5 g. 2,4-lutidine give 2 g. 1-(9-anthryl)-2-(4-methyl-2-pyridyl)ethylene, shiny greenish yellow needles, m. 222°, giving an orange color with H2SO4. Although III does not react with NaHSO3 it does so readily with the CH2 group in ArCH2CN. Passing HCl into 244 g. PhI, 65 g. paraformaldehyde, 33 g. 35% HCHO, and 145 g. ZnCl2, heating the mixture 5 h. on a water bath, and distilling the washed (H2O, very dilute NaOH, H2O) and dried lower layer give 100 g. p-IC6H4CH2Cl, b15 136-40°, which (92 g.) refluxed 12 h. with 31 g. KCN in the min. amount of H2O and 500 cc. Me2CO gives 65 g. p-IC6H4CH2CN, b13 172°. Refluxing 12 h. 23 g. 2,5-dimethyl-3-chloromethylthiophene, 12 g. KCN in a little H2O, and 200 cc. Me2CO gives 16 g. 2,5-dimethyl-3-thienylacetonitrile, b15

L6 ANSWER 143 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
180-5°. Condensation of III with the appropriate ArCH2CN in warm EtOH in the presence of a few drops of 30% aq. KOH gives the corresponding α-aryl-β-(9-anthryl)acrylonitrile, 9-C14H9CH:C(CN)Ar (VI), of which the following are prepd.: Ar = Ph, m. 163°; p-MeC6H4, m. 212°; p-FC6H4, m. 206°; p-ClC6H4, m. 213°; p-BrC6H4, m. 223°; p-IC6H4, m. 225°; p-MeOC6H4, m. 212°; p-O2N-C6H4, m. 281°; 1-C10H7 (VII), m. 219°; 2-C10H7, m. 216°; 2-thienyl, m. 203°; 2,5-dimethyl-3-thienyl, m. 210°. In the same way the following α-aryl-β-(9-methyl-10-anthryl)acrylonitriles (VIII) are prepd.: Ar = Ph, m. 253°; p-MeC6H4, m. 200°; p-IC6H4, m. 202°; p-ClC6H4, m. 240°; p-BrC6H4, m. 231°; p-MeOC6H4, m. 236°; p-O2NC6H4, m. 293°; 2-C10H7, (IX), m. 206; 2-thienyl, m. 196°. All VI and VIII are yellow to orange needles and give intense green or brownish green colors with H2SO4, except VII and IX, which give a deep red and a violet color, resp. Shaking equimol. amts. of III and PhCOMe in the presence of a few drops of 20% NaOH gives 85% 9-anthrylideneacetophenone, fine orange-yellow prisms, m. 120°, giving a deep green color with H2SO4; 9-anthrylidene-p-chloroacetophenone, yellow leaflets, m. 132°, giving a green color with H2SO4; p-iodo analog, fine orange needles, m. 168°, giving a blue color in H2SO4; 9-anthrylidene-2-acetothienone, long, shiny orange-yellow prisms, m. 162°, giving a dark green color; 9-anthrylidene(5-bromo-2-acetothienone), fine orange-yellow prisms, m. 139°, giving a dark green color; 9-anthrylidene-bis(5-chloro-2-acetothienone), fine pale yellow prisms, m. 146°, giving a pale, greenish yellow color. Refluxing a suspension of the thiosemicarbazone of the corresponding aldehyde with the appropriate halo fatty acid 5 h. in the presence of NaOAc gives the corresponding 10-anthraldehyde 4-keto-2-thiazolinylhydrazones (X) of which the following are prepd. (R, R', and m.p. in the order given): H, H, 355°; Et, H, 278°; Bu, H, 256°; C14H29, H, 208°; C16H23, H, 200°; H, Me, 355-7°; Et, Me, 287°; Bu, Me, 271°; C14H29, Me, 178°; C16H33, Me, 172°.

IT **726138-59-6**, 9-Anthraceneacrylonitrile, α-(p-methoxyphenyl)-
726139-52-2, 9-Anthraceneacrylonitrile, α-(p-methoxyphenyl)-10-methyl-
(preparation of)

RN 726138-59-6 CAPLUS

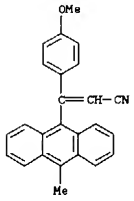
CN 9-Anthraceneacrylonitrile, α-(p-methoxyphenyl)- (5CI) (CA INDEX NAME)



L6 ANSWER 143 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)

RN 726139-52-2 CAPLUS

CN 9-Anthraceneacrylonitrile, α-(p-methoxyphenyl)-10-methyl- (5CI) (CA INDEX NAME)



L6 ANSWER 144 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1950:38078 CAPLUS
DOCUMENT NUMBER: 44:38078
ORIGINAL REFERENCE NO.: 44:7290c-i,7291a-e
TITLE: The synthesis of α,α-disubstituted succinic acids from ethyl alkylidenecyanoacetates
AUTHOR(S): Cragoe, E. J., Jr.; Robb, Charles M.; Sprague, James M.
CORPORATE SOURCE: Sharp & Dohme, Inc., Glenolden, PA
SOURCE: Journal of Organic Chemistry (1950), 15, 381-90
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 44:38078

GI For diagram(s), see printed CA Issue.

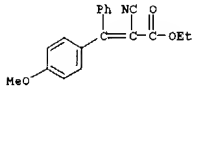
AB A study of the effect of various catalysts and solvents on the condensation of 0.5 mol. Ph2CO (I) and 0.6 mol. NCCH2CO2Et (II) shows that NaOAc, (NH4)2SO4, piperidine, Et3N, AcNH2, and C6H13CONH2 do not catalyze the reaction. With (CH2NH2)2 in PhMe 15 h. I and II give 18% Ph2C:C(CN)CO2Et (III), with NH4OAc (IV) 8 h. 42% III. Because IV is converted into the ineffective AcNH2, IV is added in small portions. In this way with 4 addns. of IV over a period of 42.5 h. I and II in C6H6 give 94% III. IV is also found to be a satisfactory catalyst for other diaryl and certain kindred ketones. The following methods are used: (A1), to 135.7 g. II, 1 mol. ketone, 48 g. AcOH, and 200 cc. C6H6 refluxed in such a way that the H2O formed is constantly removed, is added 19-62 g. (0.25-0.8 mol.) IV in 3- or 4-g. portions at 3- to 4-h. intervals, excessive amts. of IV, which otherwise will cause the formation of considerable amts. of polymeric products, being avoided; the mixture is cooled, washed with H2O, and the dried organic layer fractionally distilled; (A2), 0.75-1.2 mols. IV is used; (B1), IV is added in 1 portion; (B2), IV is added in 2 portions, the 2nd portion being added as soon as the formation of H2O ceases; (B3), IV is added in 3 portions; (B4), about 4 g. IV is added whenever the separation of H2O stops. The following RR'C:C(CN)CO2Et (V) are prepared (R, R', method, reaction time (hrs.), yield, b.p., and nD25 in the order given): Am, Am, B1, 11, 70%, b1 136-8°; C9H19, C9H19, B2, 3.5, 47% (A2, 32.5, 79%), b2 184-5°, 1.4673; Me, Ph, A2, 46, 71%, b2 134-5°, 1.5468; Et, Ph, B1, 3, 41% (A1, 32, 78%), b2 138-40°, 1.5353; Am, Ph, B3, 3, 39% (A1, 32, 87%), b2 161-3°, 1.5239; C7H15, Ph, B2, 4.5, 52% (A1, 42, 86%), b0.08 170-7°, 1.5173; C11H23, Ph, B2, 6, 22% (A1, 24, 68%), b2 182-5°, 1.5073; CH2.(CH2)4.CHCH2CH2, Ph, B2, 4, 52% (A1, 32.5, 75%), b1 174-7°, 1.5371; CH2.(CH2)4.CH(CH2)5, Ph, B2, 6.5, 29% (A1, 26.5, 67%), b0.1 190-5°, 1.5260; C6H13, p-BuC6H4, B2, 4, 14% (A1, 52, 34%), b1 180-5°, 1.5159; Et, p-HOC6H4, A1, 45, 45%, b0.1 185-8°, m. 92-3.5°; Am, o-HOC6H4, B3, 11, 28% (A1, 80, 64%), b0.4 188-90°, m. 94-5°; PhCH2CH2, PhCH2CH2, B2, 4, 68% (A1, 10, 73%), b0.1 184-7°, 1.5565; Ph, Ph, B4, 13.5, 41.7% (A1, 42.5, 84%), b1 175-82°, m. 95-7°; Ph, p-ClC6H4, A1, 42.5, 81.7%, b0.15 160-80°, m. 110-11°; p-ClC6H4, p-ClC6H4, B3, 6.5, 31.5% (A1, 51, 43.5%), b0.13 185-92°, m. 88-9°, in addition to 13% (p-ClC6H4)2C:C(CN)CONH2, m. 189-91°; o-ClC6H4, p-ClC6H4, B3, 6.3, 4.3% (A1, 92, 46%), b0.18 190-5°, m. 105-6°; Ph, p-MeOC6H4, A1, 32, 75%, b0.075 187°; Ph, thienyl, B3, 5, 8.8% (A1, 47, 53%), b2 185-8°, m. 77-8°; fluorenone, A1, 22, 87%, b0.09 194-6°, m. 58-60°; camphor, A2, 69, 37%, b0.05 121-2°, m. 86-7°; pinacolone, A2, 80.5, 13.2%, b12 127-30°, nD25 1.4680. V (R = R' = Ph) (118.5 g.) treated in 180 cc. warm EtOH with 58.5 g. KCN in 180 cc. H2O, and the mixture heated 15 min. on a steam bath, cooled, and acidified, gives 90% Ph2C(CN)CH(CN)CO2Et (VI), m. 89-91°. VI (116.3 g.) is heated

L6 ANSWER 144 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
gently with 475 g. concd. H2SO4, 380 cc. AcOH, and 95 cc. H2O until the initial vigorous evolution of CO2 ceases, the mixt. refluxed 12 h., cooled, poured onto ice, the ppt. resulting refluxed 72 h. with 20% KOH, and the mixt. acidified, giving 97% α,α-diphenylsuccinic acid, m. 175° (anhydride, prepd. with SOCl2 in 95% yield, m. 90.5-1.5°). In a similar way the following HO2CCRR'CH2CO2H (VII) (a) or CO.CRR'.CH2.CO.O (b) are prepd. (R, R', yield, b.p., and nD25 in the order given): Am, Am, b, 63%, b1.5 134-5°, 1.4537; C9H19, C9H19, b, 41%, b1 186-92°, 1.4625; Et, Ph, a, 77%, m. 149-50°; Am, Ph, b, 65%, b1 162°, 1.5159; C7H15, Ph, b, 56%, b2 170-2°, 1.5081; C11H23, Ph, b, 48%, b1-2 193-6°, 1.5010; CH2.(CH2)4.CHCH2CH2, Ph (VIII), b, 52%, b1-2 185-8°, 1.5301; CH2.(CH2)4.CH(CH2)5, Ph, b, 45%, b1-2 210°, 1.5210; C6H13, p-Bu-C6H4, b, 54%, b1-2 178-80°, m. 95-8°, 1.5055; PhCH2CH2, PhCH2CH2, a, 16%, m. 155-6°; Ph, p-ClC6H4, a, 82%, m. 187-80°; p-ClC6H4, o-ClC6H4, a, 47%, m. 195-6°; p-ClC6H4, p-ClC6H4, a, 76%, m. 188-9°. CH2.(CH2)4.CHCH2CH2CPh:C(CN)CO2Et (61 g.) is heated 15 min. in 80 cc. EtOH with 25.5 g. KCN, and the cooled mixt. dild. with 100 cc. H2O, acidified, and extd. with C6H6, giving 99% Et 2,3-dicyano-5-cyclohexyl-3-phenylpentanoate (IX). IX refluxed with 248 g. concd. H2SO4, 262 cc. AcOH, and 50 cc. H2O gives 94% VII (R = Ph, R' = CH2.(CH2)4.CHCH2CH2), m. 100-10°, which refluxed 2 h. with AcCl gives 52% VIII.

IT **14442-38-7**, Cinnamic acid, α-cyano-p-methoxy-β-phenyl-, ethyl ester
(preparation of)

RN 14442-38-7 CAPLUS

CN 2-Propenoic acid, 2-cyano-3-(4-methoxyphenyl)-3-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



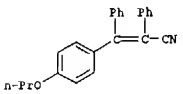
L6 ANSWER 145 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1949:38850 CAPLUS
DOCUMENT NUMBER: 43:38850
ORIGINAL REFERENCE NO.: 43:7006h-i,7007a-f
TITLE: New substituted α,β,β-triarylethylenes
AUTHOR(S): Buu-Hoi; Nguyen-Hoan; Lecocq, J.; de Clercq, M.
SOURCE: Recueil des Travaux Chimiques des Pays-Bas et de la Belgique (1948), 67, 795-812
CODEN: RTCPB4; ISSN: 0370-7539
DOCUMENT TYPE: Journal
LANGUAGE: French

AB cf. C.A. 42, 3320f. The compds. are synthesized to test for estrogenic activity. 2,4-Me2C6H3COPh (I), b12 178-80°, is prepared from m-Me2C6H4, BzCl, and AlCl3 in cold CS2. If the mixture is heated, a mixture of isomers which cannot be separated is formed. PhCH2CN in dry Et2O is treated with NaNH2, which must be freshly prepared Addition of I to the resulting Na salt gives α,β-diphenyl-β-(2,4-dimethylphenyl)acrylonitrile (II), m. 134°. Similarly, the 2,5-isomer of I, b15 184-50°, gives the β-2,5-isomer of II, m. 133°. Heating this with KOH gives the acrylamide, m. about 203-4°. Benzoylpseudocumene, b10 185°, gives α,β-diphenyl-β-(trimethylphenyl)-acrylonitrile, b10>230°. (PhCH2)2 and BzCl give 4-benzoylbibenzyl, b15 260-80°, which forms α,β-diphenyl-β-(4-phenethylphenyl)acrylonitrile b12 295-320°. The corresponding amide does not crystallize. By analogous reactions the following acrylonitriles are obtained: α,β-diphenyl-β-4-propoxyphenyl, crystallized from AcOH, m. 129-30° (A form) (the stereoisomeric B form, m. 105°, is isolated from the mother liquors); α,β-diphenyl-β-(4-butoxyphenyl), m. 114°; α,β-diphenyl-β-(2-methyl-4-methoxyphenyl), b14 255-65°, m. 134-5°; α,β-diphenyl-β-1-naphthyl, from which the known cis isomer, m. 176-8°, and the new trans isomer, b1 230-50°, m. about 129-30°, are separated; α,β-diphenyl-β-(4-methoxy-1-naphthyl), m. 166-7°; α,β-diphenyl-β-2-naphthyl, m. 180-1°; α-(p-methoxyphenyl)-β-phenyl-β-2-naphthyl, m. 202°; α,β-diphenyl-β-(6-methoxy-2-naphthyl), A form (cis?) m. 160°, B form m. 146°; α-(p-methoxyphenyl)-β-phenyl-β-(6-ethoxy-2-naphthyl), m. 185°; α,β-diphenyl-β-(5,6,7,8-tetrahydro-2-naphthyl), form A m. 128-30°, form B m. 140-1°; α-phenyl-β-(p-methoxyphenyl)-β-(5,6,7,8-tetrahydro-2-naphthyl) (from 2-p-anisoyl-5,6,7,8-tetrahydronaphthalene, b15 275-80°, m. 86°), A form m. 184°, B form m. 171°; α,β-diphenyl-β-5-acenaphthenyl, form A m. 232°, form B m. 194°; α,β-diphenyl-β-4-biphenylyl, form A m. 210° (amide m. 243°), form B m. 184°; α-phenyl-β-(o-chlorophenyl)-β-4-biphenylyl, b30 340-60°, m. 177° [from 4-(o-chlorobenzoyl)biphenyl, m. 94°]. The usual Friedel-Crafts reaction also gives 5-p-anisoylacenaphthene, b15 295-305°, m. 81°, and 5-o-chlorobenzoylacenaphthene, b12 275-6°, m. 146°. Attempts to form acrylonitriles from 2-benzoylthiophene, 3-benzoyl-2,5-thioxene, and 2-benzoylfuran were unsuccessful. p-PhCH2COC6H4OMe with 1-ClOH7MgBr gives a carbinol which dehydrates over 98% HCO2H to 1-phenyl-2-(p-methoxyphenyl)-2-(1-naphthyl)ethene, b12 295-310°, m. 102° (1-Br derivative, becomes

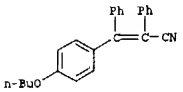
L6 ANSWER 145 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
a transparent resin about 80°). In the same way are prepd. 1-phenyl-2-(p-methoxyphenyl)-2-(5-acenaphthenyl)ethylene, b13 325°, m. 118-19° (1-Br deriv., becomes a resin below 102°); 1-phenyl-2-(p-methoxyphenyl)-2-(4-biphenylyl)ethylene m. 102° (1-Br deriv., m. 138-40°). 4-(2-Furoyl)biphenyl, b13 250-2°, m. 76°, with PhCH2MgCl gives 1-phenyl-2-(2-furyl)-2-(4-biphenylyl)ethylene, b13 285-300°, m. 87°. p-NH2C6H4COPh and (AcCH2)2 give 4-(2,5-dimethyl-1-pyrryl)benzophenone, b13 239-40°, m. 133°, which with PhCH2MgCl gives 1,2-diphenyl-2-[4-(2,5-dimethyl-1-pyrryl)phenyl]ethylene, b13 270°, m. 150-2°. 1,2-Diphenyl-2-(3-thianaphthenyl)ethylene, b13 267-70°. All these compds. give colors with concd. H2SO4.

IT **721917-64-2**, Acrylonitrile, 2,3-diphenyl-3-p-propoxyphenyl-
721917-65-3, Acrylonitrile, 3-(p-butoxyphenyl)-2,3-diphenyl-
(preparation of)

RN 721917-64-2 CAPLUS
CN Acrylonitrile, 2,3-diphenyl-3-p-propoxyphenyl- (5CI) (CA INDEX NAME)



RN 721917-65-3 CAPLUS
CN Acrylonitrile, 3-(p-butoxyphenyl)-2,3-diphenyl- (5CI) (CA INDEX NAME)



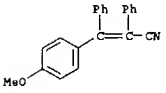
L6 ANSWER 146 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1947:30997 CAPLUS
DOCUMENT NUMBER: 41:30997
ORIGINAL REFERENCE NO.: 41:6195c-i,6196a-b
TITLE: Some α,β,β-triarylacrylonitriles, α,β,β-triarylacrylic acids, and their derivatives
AUTHOR(S): Buu-Hoi; Lecocq, Jean
CORPORATE SOURCE: Ecole polytech., Paris
SOURCE: Journal of the Chemical Society, Abstracts (1947) 641-4
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Ph2C:CPhCN (Bodroux, C.A. 5, 3683) (5 g.), 15 g. NaOH, and 15 g. iso-AmOH containing a few drops H2O, refluxed 72 hrs., give 1.5 g. Ph2C:CPhCO2H, m. 213°. p-MeC6H4CPh:CPhCN (3.1 g.), 10 g. NaOH, and 35 g. iso-AmOH, heated 1 hr., give 3 g. α,β-diphenyl-β-(p-tolyl)acrylic acid, m. 208-10°. p-MeC6H4CH2CN (5 g.) and 2 g. NaNH2 in 50 cc. ether, refluxed until evolution of NH3 ceases, slowly treated with 5 g. Ph2CO, and heated 1 hr., give 6 g. β,β-diphenyl-α-(p-tolyl)acrylonitrile (I), m. 153°; the amide (m. 216°) (1.1 g.) in 15 g. H2SO4, treated with 0.3 g. NaNO2 (ice cooling), the mixture kept at room temperature 24 hrs., and extracted with aqueous Na2CO3, gives 0.5 g. β,β-diphenyl-α-(p-tolyl)acrylic acid, m. 237-8°; it gives an intense green color with H2SO4, changing rapidly to violet and finally red. m-MeC6H4CH2CN (7 g.) similarly gives 5 g. of the m-tolyl isomer of I, m. 122°; the amide m. 177°. p-MeC6H4CH2CN (6.7 g.) and 8 g. p-MeC6H4Bz give β-phenyl-α,β-di-p-tolylacrylonitrile, b3.5 235°, m. 114-15°; the amide m. 237°. PhCH2CN (7.6 g.) and 10 g. p-ClC6H4Bz give 10 g. (probably trans) α,β-diphenyl-β-(p-chlorophenyl)acrylonitrile, pale yellow, m. 139-40°. p-MeC6H4CH2CN (8.5 g.) and 10 g. p-ClC6H4Bz give 10 g. β-phenyl-β-(p-chlorophenyl)-α-(p-tolyl)acrylonitrile, bright yellow, b4 245°, m. 147-8°; the amide m. 197°. PhCH2CN(6 g.),2.5g. NaNH2, and 8.7 g. p-MeOC6H4Bz in ether, heated 2 hrs. and the precipitate resulting on pouring into ice water crystallized from AcOH, give 9 g. cis-α,β-diphenyl-β-(p-methoxyphenyl)acrylonitrile (II), pale yellow, m. 166°; the filtrate yields 1 g. of the trans isomer (III), m. 124-5°; the ratio of II:III depends on the quality of the NaNH2 used (an old specimen gave only III); when heated in vacuo II yields III, b4 245°. II (2.5 g.) and 7.5 g. NaOH in 25 cc. aqueous AmOH, heated 3 hrs., give cis-α,β-diphenyl-β-(p-methoxyphenyl)acrylamide, yellow, m. 196-8°; trans isomer, yellow, m. 176-80°. Freshly distilled p-MeOC6H4CH2CN (6 g.) reacts slowly with active NaNH2 (2 g.) and the mixture was heated 3 hrs. after evolution of NH3 ceased; addition of 5 g. Ph2CO and refluxing an addnl. hr. gave 5 g. β,β-diphenyl-α-(p-methoxyphenyl)acrylonitrile, yellow, m. 149°; the amide m. 198°. p-MeOC6H4CH2CN (7.5 g.) and 7 g. p-MeOC6H4Bz give 7.5 g. trans-β-phenyl-α,β-di(p-methoxyphenyl)acrylonitrile, pale yellow, b4.5 260°, m. 122-5°; trans-amide, yellow, m. 243°. PhCH2CN (6 g.) and 10 g. (p-MeO-C6H4)2CO give 10 g. α-phenyl-β,β-di(p-methoxyphenyl)-acrylonitrile (IV), pale yellow, m. 159°; 7 g. IV, 21 g. NaOH, and 70 g. aqueous AmOH, refluxed 3 hrs., give the amide, m. 209°; heating 3 days gives the acid, m. 169° (Koelsch, C.A. 26, 3790). p-MeC6H4CH2CN (6.7 g.) and 10 g. (p-MeOC6H4)2CO give 7 g. α-(p-tolyl)-β,β-bis-(p-methoxyphenyl)acrylonitrile, m. 110-11° (much unchanged ketone

L6 ANSWER 146 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN (Continued)
recovered); H2SO4 gives a deep violet color; amide, yellow, m. 213°. PhCH2CN (7.6 g.) and 11.2 g. 3,4-(MeO)2C6H3Bz give 8 g. cis-α,β-diphenyl-β-(3,4-dimethoxyphenyl)acrylonitrile, yellow, m. 181°, and 2 g. of the trans isomer, m. 143-5°; both isomers give the same (trans?) amide, yellow, m. 198°. PhCH2CN (7 g.) and 10 g. 2,4-(MeO)2C6H3Bz give 6 g. α,β-diphenyl-β-(2,4-dimethoxyphenyl)acrylonitrile, yellow, b0.4 235°, m. 146-8°. PhCH2CN (9.2 g.) and 15 g. Michler's ketone give 0.5 g. α-phenyl-β,β-bis(p-dimethylaminophenyl)-acrylonitrile, deep yellow, m. 185°. Fluorenone and anthraquinone do not yield nitriles by this method. Many of these compds. are rather estrogenic and are now under test for other physiol. properties.

IT **35363-69-0**, Acrylonitrile, 3-(p-methoxyphenyl)-2,3-diphenyl-
(preparation of)

RN 35363-69-0 CAPLUS
CN Benzeneacetonitrile, α-[(4-methoxyphenyl)phenylmethylene]- (9CI) (CA INDEX NAME)



=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	698.48	880.62

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-102.20	-102.20

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L6 ANSWER 63 OF 146 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:651232 CAPLUS
DOCUMENT NUMBER: 117:251232
TITLE: Electrocyclic aromatic substitution by nitrile ylides to give 3H-2-benzazepines: substituent effects and mechanism
AUTHOR(S): Groundwater, Paul W.; Sharp, John T.
CORPORATE SOURCE: Dep. Chem., Univ. Edinburgh, Edinburgh, EH9 3JJ, UK
SOURCE: Tetrahedron (1992), 48(37), 7951-64
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 117:251232
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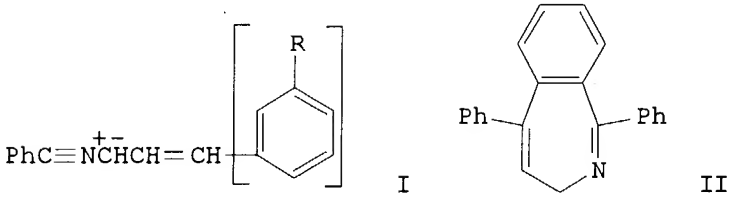

I

II

AB Benzonitrile 3,3-diarylallyl ylides I (R = H, Me, OMe, Cl, CF3), generated by the base-induced dehydrochlorination of imidoyl chlorides, cyclized by 1,7-ring closure to give 3H-2-benzazepines e.g., II, in contrast to analogous diazo-compds. which prefer 1,5-electrocyclization. Asym. placed substituents [R in I] favor substitution at the ortho (2') position irresp. of their polar electronic effects. Deuterium labeling studies have shown that the cyclization step is irreversible for these nitrile ylides in contrast to the analogous diazo-compds., for which it is reversible.

IT **144617-66-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and sequential reduction and N-benzoylation of)

RN 144617-66-3 CAPLUS
CN 2-Propenenitrile, 3,3-bis(3-methoxyphenyl)- (9CI) (CA INDEX NAME)